

A framework of the harmonic Arnoldi method for evaluating φ -functions with applications to exponential integrators

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Abstract

In recent years, a great deal of attention has been focused on numerically solving exponential integrators. The important ingredient to the implementation of exponential integrators is the efficient and accurate evaluation of the so called φ -functions on a given vector. The Krylov subspace method is an important technique for this problem. For this type of method, however, restarts become essential for the sake of storage requirements or due to the growing computational complexity of evaluating the matrix function on a Hessenberg matrix of growing size. Another problem in computing φ -functions is the lack of a clear residual notion. The contribution of this work is threefold. First, we introduce a framework of the harmonic Arnoldi method for φ -functions, which is based on the residual and the oblique projection technique. Second, we establish the relationship between the harmonic Arnoldi approximation and the classical Arnoldi approximation, and compare the harmonic Arnoldi method with the Arnoldi method from a theoretical point of view. Third, we apply the thick-restarting strategy to the harmonic Arnoldi method, and propose a thick-restated harmonic Arnoldi algorithm for evaluating φ -functions. An advantage of the new algorithm is that we can compute several φ -functions simultaneously in the same search subspace. We show the merit of augmenting approximate eigenvectors in the search subspace, and give insight into the relationship between the error and the residual of φ -functions. Numerical experiments show the superiority of our new algorithm over many state-of-the-art algorithms for the computation of φ -functions.

Keywords: Exponential integrators, φ -functions, Matrix exponential, Harmonic Arnoldi method, Oblique projection method, Thick-restarting strategy.

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1 Introduction

Exponential integrators have been employed in various large scale computations [27, 33], such as reaction-diffusion systems [17], mathematical finance [53], classical and quantum-classical molecular dynamics [55], Schrödinger equations [5], Maxwell equations [7], regularization of ill-posed problems [30], and so on. The key to the implementation of exponential integrators is the efficient and accurate evaluation of the matrix exponential and other φ -functions. These φ -functions are defined for scalar arguments by the integral representation

$$\varphi_0(z) = e^z \quad \text{and} \quad \varphi_\ell(z) = \frac{1}{(\ell-1)!} \int_0^1 e^{(1-\theta)z} \theta^{\ell-1} d\theta, \quad \ell = 1, 2, \dots, \quad z \in \mathbb{C}, \quad (1.1)$$

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moreover, these φ -functions satisfy the following recurrence relation

$$\varphi_\ell(z) = z\varphi_{\ell+1}(z) + \frac{1}{\ell!}, \quad \ell = 0, 1, 2, \dots \quad (1.2)$$

The definition can be extended to matrices instead of scalars using any of the available definitions of matrix functions [33, 48].

Exponential integrators constitute an interesting class of numerical methods for the time integration of stiff systems of differential equations. The so-called φ -functions and their evaluation are crucial for stability and speed of exponential integrators. The important ingredient to implementation of exponential integrators is the computation of the matrix exponential and related φ -functions on a given vector [33, 48]. In some practical applications, it is required to compute a few φ -functions on a given vector [33]

$$\mathbf{y}(t) = \varphi_\ell(-tA)\mathbf{v}, \quad \ell = 0, 1, \dots, s, \quad (1.3)$$

where A is a large scale matrix and $s \geq 0$ is a user-prescribed parameter. In this paper, we assume that $-tA$ is semi-negative definite, i.e., the real part of the spectrum of $-tA$ lies in the left half plane, and we are interested in solving the $(s + 1)$ vectors *simultaneously* in the *same* search subspace.

Recently, a great deal of attention has been focused on numerical solution of exponential integrators. For instance, a MATLAB package called EXPINT [6] is provided which aims to facilitate the quick deployment and testing of exponential integrators. This approach is based on a modification of the scaling and squaring technique for the matrix exponential [27, 28, 58], and is suitable for φ -functions of medium sized matrices. In [56], Schmelzer and Trefethen show that the φ -functions can be evaluated by using rational approximations constructed via Carathéodory-Fejér approximation or contour integrals. In [48], an adaptive Krylov subspace algorithm is proposed for evaluating the φ -functions appearing in exponential integrators. The *phimp* function is given for calculating the action of linear combinations of φ_ℓ on operand vectors, and it can be considered as an extension of the codes provided in EXPOKIT [57]. We refer to the review paper [33] and the references therein for the properties of exponential integrators and some efficient numerical methods for solving them.

The Krylov subspace methods are popular techniques for the computation of φ -functions [20, 21, 22, 27, 31, 32, 33, 47, 48, 53, 64], in which the Arnoldi method is a widely used one [47, 48, 54, 57]. In this method, the large matrix A is projected into a much smaller subspace, then the matrix function is applied to the reduced matrix (or the projection matrix), and finally the approximation is projected back to the original large space. However, the maximum number of iterations that can be performed is often limited by the storage requirements of the full Arnoldi basis. A further limiting factor is the growing orthogonalization cost of computing the Arnoldi basis and the cost of evaluating the matrix function of the projection matrix for larger values of Arnoldi steps.

In order to overcome these difficulties, several alternative approaches have also been proposed. The first one is to use other subspaces with superior approximation properties, such as the extended Krylov subspace methods [13, 21, 37] or the shift-and-invert Krylov subspace methods [22, 43, 39, 44, 53, 62]. Both of them can be viewed as special cases of the rational Krylov subspace methods [4, 22, 24, 25, 49], with the aim to reach a targeted accuracy within significantly fewer iterations. However, the rational Krylov subspace methods require to solve a (shifted) linear system at each Arnoldi step, which is a major drawback for situations when A is large or the matrix is not explicitly available but only implicitly as a routine returning matrix-vector products.

The other possible approach for circumventing the problems mentioned above is based on restarting. The restarted Krylov subspace methods [1, 2, 14, 15, 34, 60] restart the Arnoldi process periodically, to

avoid storing large sets of Arnoldi basis vectors. In [15], a deflated restarting technique was proposed to accelerate the convergence of the restarted Arnoldi approximation. Its effect is to ultimately deflate a specific invariant subspace of the matrix which most impedes the convergence of the restarted Arnoldi approximation process. Recently, Frommer *et al.* utilized an integral representation for the error of the iterates in the Arnoldi method, and developed a quadrature-based algorithm with deflated restarting [18]. However, as was pointed out in [18], none of the restarting approaches for general matrix functions was completely satisfactory until now. For instance, all of these variants may solve the storage problem for the Arnoldi basis, but still have to suffer from operating complexity, growing cost per restart cycle [15], numerical instability [34], and so on.

Another difficulty arises in the computation of matrix functions is the lack of a clear residual notion. The residual can provide a reliable stopping criterion, moreover, it can be used to restart the iterative methods. For the matrix exponential function in connection with Krylov approximation, the residual expression can be found in [8, 11, 31]. In [10], one can find a discussion of the residual for the φ_1 function with respect to a Krylov approximation. Recently, Kandolf *et al.* [36] considered a residual-based error estimate for Leja interpolation of φ -functions.

In recent years, special attention has been paid to the harmonic Arnoldi method for matrix functions. In [29], Hochbruck and Hochstenbach reviewed three different derivations of the harmonic Ritz approach for matrix functions. The idea behind the harmonic Ritz approximation is that for some functions, a particular target may be important [29]. More precisely, it is desirable to deflate some eigenvalues close to a given shift, so that the convergence speed can be improved [15, 19]. In [10], the harmonic Ritz approach was applied to the computation of φ_1 matrix function. The harmonic Ritz approach was investigated in [19] for the convergence of restarted Krylov subspace method for Stieltjes functions of matrices. To our best knowledge, however, the relation between the harmonic Arnoldi approximation and the Arnoldi approximation is still unknown.

In this paper, we investigate the residual of the φ -functions, and introduce a harmonic Arnoldi method for (1.3) that is based on the residual and the oblique projection technique. Second, we establish the relationship between the harmonic Arnoldi approximation and the classical Arnoldi approximation, and compare the harmonic Arnoldi method with the Arnoldi method from a theoretical point of view. Furthermore, we apply the thick-restarting strategy [65] to the harmonic Arnoldi method, and propose a thick-restarted harmonic Arnoldi algorithm for evaluating the φ -functions. An advantage of this new algorithm is that one can evaluate the $(s+1)$ vectors in (1.3) *simultaneously*, and solve them in the *same* search subspace. We show the merit of augmenting approximate eigenvectors in the thick-restarting strategy, and give insight into the relation between the error and the residual of the harmonic Arnoldi approximation. Numerical experiments show the efficiency of our new algorithm and its superiority over many state-of-the-art algorithms for φ -functions.

This paper is organized as follows. In section 2, we briefly introduce the Arnoldi method and shift-and-invert Arnoldi method for the computation of φ -functions. In section 3, we focus on the harmonic Arnoldi method and investigate the relationship between the harmonic Arnoldi approximation and the classical Arnoldi approximation. Moreover, we propose a thick-restarted harmonic Arnoldi algorithm which can be used to solve the $(s+1)$ vectors in (1.3) simultaneously. The relationship between the error and the residual of the harmonic Arnoldi approximation is derived in section 4. In Section 5, we show the advantage of augmenting approximate eigenvectors in the search subspace of a Krylov subspace method. Numerical experiments are reported in Section 6.

2 The Arnoldi and the shift-and-invert Arnoldi methods for φ -functions

In this section, we briefly introduce the Arnoldi method and the shift-and-invert Arnoldi method for φ -functions, and investigate the residuals of the approximations obtained from these two approaches. We show that the Arnoldi method is an orthogonal projection method, while the shift-and-invert Arnoldi method is an oblique projection method.

2.1 The Arnoldi and the shift-and-invert Arnoldi methods for matrix exponential

In this subsection, we consider the action of the φ_0 matrix function (or the matrix exponential) on a given vector

$$\mathbf{y}(t) = \varphi_0(-tA)\mathbf{v} = \exp(-tA)\mathbf{v}.$$

Let $\mathbf{v}_1 = \mathbf{v}/\|\mathbf{v}\|_2$, then in exact arithmetic, the k -step Arnoldi process will generate an orthonormal basis $V_{k+1} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{k+1}]$ for the Krylov subspace $\mathcal{K}_{k+1}(A, \mathbf{v}_1) = \text{span}\{\mathbf{v}_1, A\mathbf{v}_1, \dots, A^k\mathbf{v}_1\}$. The following Arnoldi relation holds [59]

$$AV_k = V_k H_k + h_{k+1,k} \mathbf{v}_{k+1} \mathbf{e}_k^H, \quad (2.1)$$

where H_k is a k -by- k upper-Hessenberg matrix, $\mathbf{e}_k \in \mathbb{R}^k$ is the k -th column of the identity matrix, and $(\cdot)^H$ denotes the conjugate transpose of a vector or matrix. The Arnoldi method makes use of [54]

$$\mathbf{y}_k(t) = V_k \exp(-tH_k) \beta \mathbf{e}_1 \equiv V_k \mathbf{u}_k(t),$$

as an approximation to $\mathbf{y}(t)$, where $\mathbf{u}_k(t) = \exp(-tH_k) \beta \mathbf{e}_1$ and $\beta = \|\mathbf{v}\|_2$. Notice that $\mathbf{u}'_k(t) = -H_k \mathbf{u}_k(t)$ and $\mathbf{u}_k(0) = \beta \mathbf{e}_1$, thus

$$\mathbf{y}'_k(t) = V_k \mathbf{u}'_k(t) = -V_k H_k \exp(-tH_k) \beta \mathbf{e}_1.$$

It follows from (2.1) that the residual is [8]

$$\mathbf{r}_k(t) = -A\mathbf{y}_k(t) - \mathbf{y}'_k(t) = -h_{k+1,k} \left[\mathbf{e}_k^H \exp(-tH_k) \beta \mathbf{e}_1 \right] \mathbf{v}_{k+1}, \quad (2.2)$$

and

$$\|\mathbf{r}_k(t)\|_2 = \left| h_{k+1,k} \left[\mathbf{e}_k^H \exp(-tH_k) \beta \mathbf{e}_1 \right] \right|.$$

We see from (2.2) that the residual vector $\mathbf{r}_k(t)$ is colinear with the $(k+1)$ -th basis vector \mathbf{v}_{k+1} , and it is orthogonal to the search space $\text{span}\{V_k\}$, i.e.,

$$\begin{cases} \mathbf{y}_k(t) = V_k \exp(-tH_k) \beta \mathbf{e}_1 \in \text{span}\{V_k\}, \\ -A\mathbf{y}_k(t) - \mathbf{y}'_k(t) \perp \text{span}\{V_k\}. \end{cases} \quad (2.3)$$

Thus, the Arnoldi method for matrix exponential is an orthogonal projection method [8, 59].

In recent works on the approximations of matrix functions by Krylov subspace methods, it becomes more and more apparent that the shift-and-invert Arnoldi method works tremendously better than the standard Arnoldi method [22, 43, 39, 44, 53, 62]. In this type of method, the Krylov subspace is generated by using the matrix $(I + \gamma A)^{-1}$ instead of A , where γ is a user-described parameter. Let $\tilde{\mathbf{v}}_1 = \mathbf{v}/\|\mathbf{v}\|_2$,

then in exact arithmetic, the k -step shift-and-invert Arnoldi process generates an orthonormal basis \tilde{V}_{k+1} for the Krylov subspace $\mathcal{K}_{k+1}((I + \gamma A)^{-1}, \tilde{\mathbf{v}}_1) = \text{span}\{\tilde{\mathbf{v}}_1, (I + \gamma A)^{-1}\tilde{\mathbf{v}}_1, \dots, [(I + \gamma A)^{-1}]^k \tilde{\mathbf{v}}_1\}$, and we have the following relation

$$(I + \gamma A)^{-1}\tilde{V}_k = \tilde{V}_k \tilde{H}_k + \tilde{h}_{k+1,k} \tilde{\mathbf{v}}_{k+1} \mathbf{e}_k^H, \quad (2.4)$$

where \tilde{H}_k is a k -by- k upper-Hessenberg matrix. If \tilde{H}_k is nonsingular, we denote $B_k = \frac{\tilde{H}_k^{-1} - I}{\gamma}$, then the shift-and-invert Arnoldi method uses

$$\tilde{\mathbf{y}}_k(t) = \tilde{V}_k \exp(-tB_k) \beta \mathbf{e}_1 \equiv \tilde{V}_k \tilde{\mathbf{u}}_k(t)$$

as an approximation to the desired solution, where $\tilde{\mathbf{u}}_k(t) = \exp(-tB_k) \beta \mathbf{e}_1$.

Rewrite the relation (2.4) as

$$A\tilde{V}_k = \tilde{V}_k B_k - \frac{\tilde{h}_{k+1,k}}{\gamma} (I + \gamma A) \tilde{\mathbf{v}}_{k+1} \mathbf{e}_k^H \tilde{H}_k^{-1}, \quad (2.5)$$

then we have that

$$A\tilde{\mathbf{y}}_k(t) = A\tilde{V}_k \tilde{\mathbf{u}}_k(t) = \left[\tilde{V}_k B_k - \frac{\tilde{h}_{k+1,k}}{\gamma} (I + \gamma A) \tilde{\mathbf{v}}_{k+1} \mathbf{e}_k^H \tilde{H}_k^{-1} \right] \exp(-tB_k) \beta \mathbf{e}_1,$$

and

$$\tilde{\mathbf{y}}'_k(t) = -\tilde{V}_k B_k \exp(-tB_k) \beta \mathbf{e}_1.$$

So the residual can be expressed as [8]

$$\tilde{\mathbf{r}}_k(t) = -A\tilde{\mathbf{y}}_k(t) - \tilde{\mathbf{y}}'_k(t) = \frac{\tilde{h}_{k+1,k}}{\gamma} \left[\mathbf{e}_k^H \tilde{H}_k^{-1} \exp(-tB_k) \beta \mathbf{e}_1 \right] (I + \gamma A) \tilde{\mathbf{v}}_{k+1}, \quad (2.6)$$

and

$$\|\tilde{\mathbf{r}}_k(t)\|_2 = \left| \frac{\tilde{h}_{k+1,k}}{\gamma} \left[\mathbf{e}_k^H \tilde{H}_k^{-1} \exp(-tB_k) \beta \mathbf{e}_1 \right] \right| \cdot \|\tilde{\mathbf{v}}_{k+1} + \gamma A \tilde{\mathbf{v}}_{k+1}\|_2.$$

It is seen from (2.6) that the residual vector $\tilde{\mathbf{r}}_k(t)$ is colinear with $(I + \gamma A) \tilde{\mathbf{v}}_{k+1}$, and it is orthogonal to the space $\text{span}\{(I + \gamma A)^{-H} \tilde{V}_k\}$:

$$[(I + \gamma A)^{-H} \tilde{V}_k]^H \tilde{\mathbf{r}}_k(t) = \tilde{V}_k^H (I + \gamma A)^{-1} [-A\tilde{\mathbf{y}}_k(t) - \tilde{\mathbf{y}}'_k(t)] = \mathbf{0}.$$

That is,

$$\begin{cases} \tilde{\mathbf{y}}_k(t) = \tilde{V}_k \exp(-tB_k) \beta \mathbf{e}_1 \in \text{span}\{\tilde{V}_k\}, \\ -A\tilde{\mathbf{y}}_k(t) - \tilde{\mathbf{y}}'_k(t) \perp \text{span}\{(I + \gamma A)^{-H} \tilde{V}_k\}. \end{cases} \quad (2.7)$$

In other words, the shift-and-invert Arnoldi method for matrix exponential is an oblique projection method.

2.2 The Arnoldi and the shift-and-invert Arnoldi methods for φ_ℓ ($\ell \geq 1$) functions

We consider the problem of

$$\mathbf{y}(t) = \varphi_\ell(-tA) \mathbf{v}, \quad \ell = 1, 2, \dots, s. \quad (2.8)$$

Given the Arnoldi relation (2.1), the Arnoldi method uses [47, 48]

$$\mathbf{y}_{\ell,k}(t) = V_k \varphi_\ell(-tH_k) \beta \mathbf{e}_1$$

as an approximate solution to $\mathbf{y}(t)$. In this subsection, we aim to evaluate the residual of the approximation efficiently, and provide an effective stopping criterion for the computation of (2.8).

Note that $\mathbf{y}(t)$ solves the following differential equation

$$\begin{cases} \mathbf{y}'(t) = -A\mathbf{y}(t) - \frac{\ell}{t}\mathbf{y}(t) + \frac{1}{t(\ell-1)!}\mathbf{v}, \\ \mathbf{y}(0) = \mathbf{v}/\ell!. \end{cases} \quad (2.9)$$

Then we can define

$$\mathbf{r}_{\ell,k}(t) = -A\mathbf{y}_{\ell,k}(t) - \frac{\ell}{t}\mathbf{y}_{\ell,k}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \mathbf{y}'_{\ell,k}(t) \quad (2.10)$$

as a residual of $\mathbf{y}_{\ell,k}(t)$. On the other hand, we have from the relation

$$\varphi_{\ell-1}(-tA)\mathbf{v} = -tA\varphi_{\ell}(-tA)\mathbf{v} + \frac{1}{(\ell-1)!}\mathbf{v}, \quad \ell \geq 1 \quad (2.11)$$

that

$$\check{\mathbf{r}}(t) = -tAV_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 - V_k\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}V_k\beta\mathbf{e}_1 \quad (2.12)$$

can also be utilized as a residual of $\mathbf{y}_{\ell,k}(t)$. The following proposition reveals the relationship between the two residuals (2.10) and (2.12).

Proposition 2.1. *Under the above notations, we have*

$$\mathbf{r}_{\ell,k}(t) = \frac{1}{t}\check{\mathbf{r}}(t) = -h_{k+1,k}[\mathbf{e}_k^H\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1]\mathbf{v}_{k+1}, \quad (2.13)$$

and

$$\|\mathbf{r}_{\ell,k}(t)\|_2 = \left| h_{k+1,k}[\mathbf{e}_k^H\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1] \right|. \quad (2.14)$$

Proof. It follows from (2.9) that

$$\varphi'_{\ell}(-tH_k)\beta\mathbf{e}_1 = -H_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 - \frac{\ell}{t}\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{t(\ell-1)!}\beta\mathbf{e}_1.$$

Thus,

$$\begin{aligned} \mathbf{r}_{\ell,k}(t) &= -A\mathbf{y}_{\ell,k}(t) - \frac{\ell}{t}\mathbf{y}_{\ell,k}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \mathbf{y}'_{\ell,k}(t) \\ &= -AV_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 - \frac{\ell}{t}V_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 - V_k\varphi'_{\ell}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{t(\ell-1)!}\mathbf{v} \\ &= -AV_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 + V_k\left[H_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 - \frac{1}{t(\ell-1)!}\beta\mathbf{e}_1\right] + \frac{1}{t(\ell-1)!}\mathbf{v}. \end{aligned} \quad (2.15)$$

Notice from (1.2) that

$$\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 = -tH_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}\beta\mathbf{e}_1, \quad \ell = 1, 2, \dots$$

So we have

$$H_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 - \frac{1}{t(\ell-1)!}\beta\mathbf{e}_1 = -\frac{1}{t}\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1, \quad (2.16)$$

and (2.15) can be rewritten as

$$\mathbf{r}_{\ell,k}(t) = -AV_k\varphi_{\ell}(-tH_k)\beta\mathbf{e}_1 - \frac{1}{t}V_k\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{t(\ell-1)!}V_k\beta\mathbf{e}_1. \quad (2.17)$$

On the other hand,

$$\begin{aligned}
\check{\mathbf{r}}(t) &= -tAV_k\varphi_\ell(-tH_k)\beta\mathbf{e}_1 - V_k\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}V_k\beta\mathbf{e}_1 \\
&= t\left[-AV_k\varphi_\ell(-tH_k)\beta\mathbf{e}_1 - \frac{1}{t}V_k\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{t(\ell-1)!}V_k\beta\mathbf{e}_1\right] \\
&= t \cdot \mathbf{r}_{\ell,k}(t).
\end{aligned}$$

Moreover, we have from (2.1) that

$$\begin{aligned}
\check{\mathbf{r}}(t) &= -tAV_k\varphi_\ell(-tH_k)\beta\mathbf{e}_1 - V_k\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}V_k\beta\mathbf{e}_1 \\
&= -t(V_kH_k + h_{k+1,k}\mathbf{v}_{k+1}\mathbf{e}_k^H)\varphi_\ell(-tH_k)\beta\mathbf{e}_1 - V_k\varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}V_k\beta\mathbf{e}_1 \\
&= V_k\left[-tH_k\varphi_\ell(-tH_k)\beta\mathbf{e}_1 - \varphi_{\ell-1}(-tH_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}\beta\mathbf{e}_1\right] - th_{k+1,k}[\mathbf{e}_k^H\varphi_\ell(-tH_k)\beta\mathbf{e}_1]\mathbf{v}_{k+1} \\
&= -th_{k+1,k}[\mathbf{e}_k^H\varphi_\ell(-tH_k)\beta\mathbf{e}_1]\mathbf{v}_{k+1},
\end{aligned}$$

where we used (2.16); and (2.14) follows from (2.13) and the fact that $\|\mathbf{v}_{k+1}\|_2 = 1$. \square

Remark 2.1. Proposition 2.1 indicates that the residual vector $\mathbf{r}_{\ell,k}(t)$ is colinear with the $(k+1)$ -th Arnoldi basis vector \mathbf{v}_{k+1} , which is orthogonal to the search space $\text{span}\{V_k\}$, i.e.,

$$\begin{cases} \mathbf{y}_{\ell,k}(t) = V_k\varphi_\ell(-tH_k)\beta\mathbf{e}_1 \in \text{span}\{V_k\}, \\ -A\mathbf{y}_{\ell,k}(t) - \frac{\ell}{t}\mathbf{y}_{\ell,k}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \mathbf{y}'_{\ell,k}(t) \perp \text{span}\{V_k\}. \end{cases} \quad (2.18)$$

In terms of (2.3) and (2.18), the Arnoldi method for φ -functions is an orthogonal projection method.

Now we consider the shift-and-invert Arnoldi method for φ_ℓ functions with $\ell \geq 1$. Given the shift-and-invert Arnoldi relation (2.4), the shift-and-invert Arnoldi method exploits [53]

$$\tilde{\mathbf{y}}_{\ell,k}(t) = \tilde{V}_k\varphi_\ell(-tB_k)\beta\mathbf{e}_1$$

as an approximation to $\mathbf{y}(t) = \varphi_\ell(-tA)\mathbf{v}$, where $B_k = \frac{\tilde{H}_k^{-1} - I}{\gamma}$. Define

$$\tilde{\mathbf{r}}_{\ell,k}(t) = -A\tilde{\mathbf{y}}_{\ell,k}(t) - \frac{\ell}{t}\tilde{\mathbf{y}}_{\ell,k}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \tilde{\mathbf{y}}'_{\ell,k}(t), \quad (2.19)$$

we have the following result on the residual.

Proposition 2.2. Under the above notations, there holds

$$\tilde{\mathbf{r}}_{\ell,k}(t) = \frac{\tilde{h}_{k+1,k}}{\gamma} \left[\mathbf{e}_k^H \tilde{H}_k^{-1} \varphi_\ell(-tB_k)\beta\mathbf{e}_1 \right] (I + \gamma A) \tilde{\mathbf{v}}_{k+1}, \quad (2.20)$$

and

$$\|\tilde{\mathbf{r}}_{\ell,k}(t)\|_2 = \left| \frac{\tilde{h}_{k+1,k}}{\gamma} \left[\mathbf{e}_k^H \tilde{H}_k^{-1} \varphi_\ell(-tB_k)\beta\mathbf{e}_1 \right] \right| \cdot \|\tilde{\mathbf{v}}_{k+1} + \gamma A \tilde{\mathbf{v}}_{k+1}\|_2.$$

Proof. It follows from the shift-and-invert Arnoldi relation and (1.2) that

$$\begin{aligned}
t \cdot \tilde{\mathbf{r}}_{\ell,k}(t) &= -tA\tilde{V}_k\varphi_\ell(-tB_k)\beta\mathbf{e}_1 - \tilde{V}_k\varphi_{\ell-1}(-tB_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}\tilde{V}_k\beta\mathbf{e}_1 \\
&= -t\left[\tilde{V}_kB_k - \frac{\tilde{h}_{k+1,k}}{\gamma}(I + \gamma A)\tilde{\mathbf{v}}_{k+1}\mathbf{e}_k^H\tilde{H}_k^{-1}\right]\varphi_\ell(-tB_k)\beta\mathbf{e}_1 - \tilde{V}_k\varphi_{\ell-1}(-tB_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}\tilde{V}_k\beta\mathbf{e}_1 \\
&= \tilde{V}_k\left[-tB_k\varphi_\ell(-tB_k)\beta\mathbf{e}_1 - \varphi_{\ell-1}(-tB_k)\beta\mathbf{e}_1 + \frac{1}{(\ell-1)!}\beta\mathbf{e}_1\right] \\
&\quad + t\frac{\tilde{h}_{k+1,k}}{\gamma}\left[\mathbf{e}_k^H\tilde{H}_k^{-1}\varphi_\ell(-tB_k)\beta\mathbf{e}_1\right](I + \gamma A)\tilde{\mathbf{v}}_{k+1} \\
&= t\frac{\tilde{h}_{k+1,k}}{\gamma}\left[\mathbf{e}_k^H\tilde{H}_k^{-1}\varphi_\ell(-tB_k)\beta\mathbf{e}_1\right](I + \gamma A)\tilde{\mathbf{v}}_{k+1},
\end{aligned}$$

and

$$\begin{aligned}
\|\tilde{\mathbf{r}}_{\ell,k}(t)\|_2 &= \left\|\frac{\tilde{h}_{k+1,k}}{\gamma}\left[\mathbf{e}_k^H\tilde{H}_k^{-1}\varphi_\ell(-tB_k)\beta\mathbf{e}_1\right](I + \gamma A)\tilde{\mathbf{v}}_{k+1}\right\|_2 \\
&= \left|\frac{\tilde{h}_{k+1,k}}{\gamma}\left[\mathbf{e}_k^H\tilde{H}_k^{-1}\varphi_\ell(-tB_k)\beta\mathbf{e}_1\right]\right| \cdot \|\tilde{\mathbf{v}}_{k+1} + \gamma A\tilde{\mathbf{v}}_{k+1}\|_2.
\end{aligned}$$

□

Remark 2.2. Proposition 2.2 shows that the residual vector $\tilde{\mathbf{r}}_{\ell,k}(t)$ is colinear with $(I + \gamma A)\tilde{\mathbf{v}}_{k+1}$, which is orthogonal to $\text{span}\{(I + \gamma A)^{-H}\tilde{V}_k\}$, i.e.,

$$\begin{cases} \tilde{\mathbf{y}}_{\ell,k}(t) = \tilde{V}_k\varphi_\ell(-tB_k)\beta\mathbf{e}_1 \in \text{span}\{\tilde{V}_k\}, \\ -A\tilde{\mathbf{y}}_{\ell,k}(t) - \frac{\ell}{t}\tilde{\mathbf{y}}_{\ell,k}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \tilde{\mathbf{y}}'_{\ell,k}(t) \perp \text{span}\{(I + \gamma A)^{-H}\tilde{V}_k\}. \end{cases} \quad (2.21)$$

In view of (2.7) and (2.21), the shift-and-invert Arnoldi method for φ -functions is an oblique projection method. In this method, however, one has to compute $(I + \gamma A)^{-1}$ in advance, or to solve a shifted linear system in each step of the shift-and-invert Arnoldi process, which is prohibitive for large scale matrices.

3 A harmonic Arnoldi method and a thick-restarted harmonic Arnoldi algorithm for φ -functions

In order to accelerate convergence of the standard Arnoldi method, it is preferable to deflate some eigenvalues near a singularity of the function in question [15, 19, 29]. For instance, one often needs to deflate some eigenvalues close to a given shift (e.g., the smallest eigenvalues in magnitude [15, 19]), so that the convergence speed can be improved significantly. It is well known that the harmonic Arnoldi method is appropriate to interior eigenproblems [50, 59]. In [29], Hochbruck and Hochstenbach reviewed three different derivations of a harmonic Ritz approach for matrix functions: (i) using a projection onto the search space; (ii) approximating the shifted linear systems in the Dunford–Taylor integral representation; (iii) interpolating the function in certain points.

In this section, we introduce the harmonic Arnoldi method for φ -functions based on the residual and the harmonic projection technique for large eigenproblems [50, 54], and shed light on the relationship between the harmonic Arnoldi method and the standard Arnoldi method. Furthermore, we consider how to restart the harmonic Arnoldi method efficiently, by using the thick-restarting strategy that is popular

for large scale eigenproblems and linear equations [35, 46, 65]. Thanks to the residuals of the harmonic Arnoldi approximations, our new algorithm can solve (1.3) simultaneously in the same search subspace.

3.1 The harmonic Arnoldi method for matrix exponential

The Arnoldi relation (2.1) can be rewritten as

$$(I + \gamma A)V_k = V_k(I + \gamma H_k) + \gamma h_{k+1,k} \mathbf{v}_{k+1} \mathbf{e}_k^H, \quad (3.1)$$

where γ is a user-prescribed parameter. Suppose that we want to seek an approximation $\check{\mathbf{y}}_k(t) \equiv V_k \check{\mathbf{u}}_k(t)$ to $\exp[-t(I + \gamma A)^{-1}] \mathbf{v}$ in the subspace $\text{span}\{V_k\}$, and the residual is [8]

$$\check{\mathbf{r}}_k(t) = -(I + \gamma A)^{-1} \check{\mathbf{y}}_k(t) - \check{\mathbf{y}}_k'(t).$$

Now we consider how to compute $\check{\mathbf{u}}_k(t)$. Motivated by the harmonic Arnoldi method for interior eigenvalue problems [50, 59], let

$$\check{\mathbf{r}}_k(t) \perp \text{span}\{(I + \gamma A)^H(I + \gamma A)V_k\},$$

that is,

$$V_k^H(I + \gamma A)^H(I + \gamma A) \left[-(I + \gamma A)^{-1} V_k \check{\mathbf{u}}_k(t) - V_k \check{\mathbf{u}}_k'(t) \right] = \mathbf{0}. \quad (3.2)$$

If $M_k \equiv (I + \gamma H_k)^H(I + \gamma H_k) + \gamma^2 h_{k+1,k}^2 \mathbf{e}_k \mathbf{e}_k^H$ is nonsingular, denote $Q_k = M_k^{-1}(I + \gamma H_k)^H$, then we obtain from (3.2) that

$$\check{\mathbf{u}}_k'(t) = -Q_k \check{\mathbf{u}}_k(t), \quad \check{\mathbf{u}}_k(0) = \beta \mathbf{e}_1,$$

and

$$\check{\mathbf{u}}_k(t) = \exp(-tQ_k) \beta \mathbf{e}_1.$$

Thus, we can approximate $\exp[-t(I + \gamma A)^{-1}] \mathbf{v}$ by using

$$\check{\mathbf{y}}_k(t) = V_k \check{\mathbf{u}}_k(t) = V_k \exp(-tQ_k) \beta \mathbf{e}_1. \quad (3.3)$$

Denote

$$T_k = \frac{Q_k^{-1} - I}{\gamma} = H_k + \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \mathbf{e}_k^H, \quad (3.4)$$

in view of (3.3), the idea behind the harmonic Arnoldi method is to use

$$\hat{\mathbf{y}}_k(t) = V_k \hat{\mathbf{u}}_k(t) = V_k \exp(-tT_k) \beta \mathbf{e}_1 \quad (3.5)$$

as an approximation to $\mathbf{y}(t) = \exp(-tA) \mathbf{v}$, where $\hat{\mathbf{u}}_k(t) = \exp(-tT_k) \beta \mathbf{e}_1$. The residual is

$$\begin{aligned} \hat{\mathbf{r}}_k(t) &= -A \hat{\mathbf{y}}_k(t) - \hat{\mathbf{y}}_k'(t) \\ &= \left[\gamma h_{k+1,k}^2 V_k (I + \gamma H_k)^{-H} \mathbf{e}_k \mathbf{e}_k^H - h_{k+1,k} \mathbf{v}_{k+1} \mathbf{e}_k^H \right] \exp(-tT_k) \beta \mathbf{e}_1 \\ &= V_{k+1} \begin{bmatrix} \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \\ -h_{k+1,k} \end{bmatrix} \left[\mathbf{e}_k^H \exp(-tT_k) \beta \mathbf{e}_1 \right], \end{aligned} \quad (3.6)$$

and

$$\|\hat{\mathbf{r}}_k(t)\|_2 = \left\| \begin{bmatrix} \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \\ -h_{k+1,k} \end{bmatrix} \right\|_2 \cdot |\mathbf{e}_k^H \exp(-tT_k) \beta \mathbf{e}_1|.$$

Thus, the residual vector $\hat{\mathbf{r}}_k(t)$ is colinear with the residual of the harmonic Ritz pairs [50, 59], and the harmonic Arnoldi method for matrix exponential is an oblique projection method in the sense that

$$\begin{cases} \hat{\mathbf{y}}_k(t) = V_k \exp(-tT_k) \beta \mathbf{e}_1 \in \text{span}\{V_k\}, \\ -A\hat{\mathbf{y}}_k(t) - \hat{\mathbf{y}}'_k(t) \perp \text{span}\{(I + \gamma A)V_k\}. \end{cases} \quad (3.7)$$

The method is an alternative Krylov subspace approach to the Arnoldi method. Indeed, the Arnoldi approximation $\mathbf{y}_k(t)$ can be characterized as $\mathbf{y}_k(t) = q_{H_k}(A)\mathbf{v}$, where q_{H_k} interpolates the exponential function at the eigenvalues of H_k , which are the Ritz values of A with respect to the Krylov subspace $\mathcal{K}_k(A, \mathbf{v})$ [54]. Alternatively, the harmonic Arnoldi approximation $\hat{\mathbf{y}}_k(t)$ is based on polynomial interpolation at the harmonic Ritz values instead of the standard Ritz values [19].

To our best knowledge, however, the relationship between the harmonic Arnoldi method and the standard Arnoldi method is still unknown. The following theorem establishes the relationship of the approximations and residuals of the two approaches for matrix exponential.

Theorem 3.1. *Denote by $\mathbf{y}_k(t) = V_k \exp(-tH_k) \beta \mathbf{e}_1$ and $\hat{\mathbf{y}}_k(t) = V_k \exp(-tT_k) \beta \mathbf{e}_1$ the Arnoldi approximation and the harmonic Arnoldi approximation to $\mathbf{y}(t)$, respectively; and by $\mathbf{r}_k(t)$ and $\hat{\mathbf{r}}_k(t)$ the corresponding residuals. Let $\mathbf{g} = \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k$ and $k \geq 2$, then we have*

$$\hat{\mathbf{y}}_k(t) = \mathbf{y}_k(t) + \beta V_k \sum_{m=2}^{\infty} \left(\left[\frac{(-t)^m}{m!} \right] \sum_{p=1}^{m-1} [\mathbf{e}_k^H(T_k)^p \mathbf{e}_1] [(H_k)^{m-1-p} \mathbf{g}] \right), \quad (3.8)$$

and

$$\hat{\mathbf{r}}_k(t) = \mathbf{r}_k(t) - (h_{k+1,k} \alpha) \mathbf{v}_{k+1} + \gamma h_{k+1,k}^2 \left[\mathbf{e}_k^H \exp(-tH_k) \beta \mathbf{e}_1 + \alpha \right] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k, \quad (3.9)$$

where

$$\alpha = \beta \sum_{m=2}^{\infty} \left(\left[\frac{(-t)^m}{m!} \right] \sum_{p=1}^{m-1} [\mathbf{e}_k^H(T_k)^p \mathbf{e}_1] [\mathbf{e}_k^H(H_k)^{m-1-p} \mathbf{g}] \right).$$

Proof. By the definition of matrix exponential, we have

$$\mathbf{u}_k(t) = \exp(-tH_k) \beta \mathbf{e}_1 = \beta \sum_{m=0}^{\infty} \left[\frac{(-tH_k)^m}{m!} \right] \mathbf{e}_1,$$

$$\hat{\mathbf{u}}_k(t) = \exp(-tT_k) \beta \mathbf{e}_1 = \beta \sum_{m=0}^{\infty} \left[\frac{(-tT_k)^m}{m!} \right] \mathbf{e}_1,$$

and

$$\hat{\mathbf{u}}_k(t) - \mathbf{u}_k(t) = \beta \sum_{m=0}^{\infty} \left[\frac{(-t)^m}{m!} \right] [(T_k)^m \mathbf{e}_1 - (H_k)^m \mathbf{e}_1]. \quad (3.10)$$

Furthermore, for $k \geq 2$, we have from $T_k \mathbf{e}_1 = [H_k + \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \mathbf{e}_k^H] \mathbf{e}_1 = H_k \mathbf{e}_1$ that

$$\begin{aligned} \sum_{m=0}^{\infty} \left[\frac{(-t)^m}{m!} \right] [(T_k)^m \mathbf{e}_1 - (H_k)^m \mathbf{e}_1] &= \sum_{m=1}^{\infty} \left[\frac{(-t)^m}{m!} \right] [(T_k)^m \mathbf{e}_1 - (H_k)^m \mathbf{e}_1] \\ &= \sum_{m=2}^{\infty} \left[\frac{(-t)^m}{m!} \right] [(T_k)^m \mathbf{e}_1 - (H_k)^m \mathbf{e}_1]. \end{aligned}$$

Thus,

$$\begin{aligned}\widehat{\mathbf{y}}_k(t) - \mathbf{y}_k(t) &= V_k \widehat{\mathbf{u}}_k(t) - V_k \mathbf{u}_k(t) \\ &= \beta V_k \sum_{m=2}^{\infty} \left[\frac{(-t)^m}{m!} \right] \left[(T_k)^m \mathbf{e}_1 - (H_k)^m \mathbf{e}_1 \right].\end{aligned}\quad (3.11)$$

For notation simplicity, we denote

$$T_k = H_k + \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \mathbf{e}_k^H \equiv H_k + \mathbf{g} \mathbf{e}_k^H,$$

where $\mathbf{g} = \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k$. Note that T_k is a rank-one update of H_k . Next we verify that

$$(T_k)^m \mathbf{e}_1 - (H_k)^m \mathbf{e}_1 = \sum_{p=1}^{m-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{m-1-p} \mathbf{g}]. \quad (3.12)$$

Indeed, we note that

$$(T_k)^2 \mathbf{e}_1 - (H_k)^2 \mathbf{e}_1 = [\mathbf{e}_k^H T_k \mathbf{e}_1] (H_k)^0 \mathbf{g}.$$

Assume that

$$(T_k)^j \mathbf{e}_1 - (H_k)^j \mathbf{e}_1 = \sum_{p=1}^{j-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{j-1-p} \mathbf{g}], \quad j \geq 2. \quad (3.13)$$

Thus,

$$T_k \left[(T_k)^j \mathbf{e}_1 - (H_k)^j \mathbf{e}_1 \right] = (T_k)^{j+1} \mathbf{e}_1 - (H_k)^{j+1} \mathbf{e}_1 - [\mathbf{e}_k^H (H_k)^j \mathbf{e}_1] \mathbf{g}.$$

By (3.13), we obtain

$$T_k \left[(T_k)^j \mathbf{e}_1 - (H_k)^j \mathbf{e}_1 \right] = T_k \sum_{p=1}^{j-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{j-1-p} \mathbf{g}],$$

and

$$(T_k)^{j+1} \mathbf{e}_1 - (H_k)^{j+1} \mathbf{e}_1 = \sum_{p=1}^{j-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{j-p} \mathbf{g}] + \left[\sum_{p=1}^{j-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [\mathbf{e}_k^H (H_k)^{j-1-p} \mathbf{g}] + \mathbf{e}_k^H (H_k)^j \mathbf{e}_1 \right] \mathbf{g}. \quad (3.14)$$

Moreover, it follows from (3.13) that

$$\mathbf{e}_k^H (T_k)^j \mathbf{e}_1 = \sum_{p=1}^{j-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [\mathbf{e}_k^H (H_k)^{j-1-p} \mathbf{g}] + \mathbf{e}_k^H (H_k)^j \mathbf{e}_1,$$

so we arrive at

$$\begin{aligned}(T_k)^{j+1} \mathbf{e}_1 - (H_k)^{j+1} \mathbf{e}_1 &= \sum_{p=1}^{j-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{j-p} \mathbf{g}] + [\mathbf{e}_k^H (T_k)^j \mathbf{e}_1] \mathbf{g} \\ &= \sum_{p=1}^j [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{j-p} \mathbf{g}],\end{aligned}$$

and the relation (3.12) is established. Combining (3.11) and (3.12) yields

$$\begin{aligned}\widehat{\mathbf{y}}_k(t) - \mathbf{y}_k(t) &= \beta V_k \sum_{m=2}^{\infty} \left[\frac{(-t)^m}{m!} \right] \left[(T_k)^m \mathbf{e}_1 - (H_k)^m \mathbf{e}_1 \right] \\ &= \beta V_k \sum_{m=2}^{\infty} \left[\frac{(-t)^m}{m!} \right] \left(\sum_{p=1}^{m-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{m-1-p} \mathbf{g}] \right).\end{aligned}$$

In order to prove (3.9), denote

$$\alpha = \mathbf{e}_k^H \hat{\mathbf{u}}_k(t) - \mathbf{e}_k^H \mathbf{u}_k(t) = \beta \sum_{m=2}^{\infty} \left[\frac{(-t)^m}{m!} \right] \sum_{p=1}^{m-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [\mathbf{e}_k^H (H_k)^{m-1-p} \mathbf{g}],$$

and we derive from (3.6) that

$$\begin{aligned} \hat{\mathbf{r}}_k(t) &= -h_{k+1,k} [\mathbf{e}_k^H \mathbf{u}_k(t) + \alpha] \mathbf{v}_{k+1} + \gamma h_{k+1,k}^2 [\mathbf{e}_k^H \mathbf{u}_k(t) + \alpha] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k \\ &= \mathbf{r}_k(t) - (h_{k+1,k} \alpha) \mathbf{v}_{k+1} + \gamma h_{k+1,k}^2 [\mathbf{e}_k^H \exp(-tH_k) \beta \mathbf{e}_1 + \alpha] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k. \end{aligned}$$

□

3.2 A harmonic Arnoldi method for φ_ℓ ($\ell \geq 1$) functions

In this subsection, we focus on the harmonic Arnoldi method for

$$\mathbf{y}(t) = \varphi_\ell(-tA)\mathbf{v}, \quad \ell = 1, 2, \dots, s,$$

and establish the relationship between the harmonic Arnoldi approximation and the Arnoldi approximation for φ_ℓ functions with $\ell \geq 1$.

Given the Arnoldi relation (2.1), in the harmonic Arnoldi method, we make use of

$$\hat{\mathbf{y}}_{\ell,k}(t) = V_k \varphi_\ell(-tT_k) \beta \mathbf{e}_1 \equiv V_k \hat{\mathbf{u}}_{\ell,k}(t) \quad (3.15)$$

as an approximate solution to $\mathbf{y}(t)$ in the Krylov subspace $\mathcal{K}_k(A, \mathbf{v})$, where T_k is defined in (3.4). Denote by

$$\hat{\mathbf{r}}_{\ell,k}(t) = -A \hat{\mathbf{y}}_{\ell,k}(t) - \frac{\ell}{t} \hat{\mathbf{y}}_{\ell,k}(t) + \frac{1}{t(\ell-1)!} \mathbf{v} - \hat{\mathbf{y}}'_{\ell,k}(t) \quad (3.16)$$

the residual with respect to $\hat{\mathbf{y}}_{\ell,k}(t)$, we have the following result:

Proposition 3.1. *Under the above notations, we have*

$$\hat{\mathbf{r}}_{\ell,k}(t) = \frac{1}{t} \left[-tAV_k \varphi_\ell(-tT_k) \beta \mathbf{e}_1 - V_k \varphi_{\ell-1}(-tT_k) \beta \mathbf{e}_1 + \frac{1}{(\ell-1)!} V_k \beta \mathbf{e}_1 \right] \quad (3.17)$$

$$= V_{k+1} \begin{bmatrix} \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \\ -h_{k+1,k} \end{bmatrix} [\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1], \quad (3.18)$$

and

$$[(I + \gamma A)V_k]^H \cdot \hat{\mathbf{r}}_{\ell,k}(t) = \mathbf{0}. \quad (3.19)$$

Proof. The proof of (3.17) is similar to that of (2.13), and is omitted. For (3.18), it follows from (2.1), (2.11) and (3.4) that

$$\begin{aligned} & -tAV_k \varphi_\ell(-tT_k) \beta \mathbf{e}_1 - V_k \varphi_{\ell-1}(-tT_k) \beta \mathbf{e}_1 + \frac{1}{(\ell-1)!} V_k \beta \mathbf{e}_1 \\ &= -t(V_k H_k + h_{k+1,k} \mathbf{v}_{k+1} \mathbf{e}_k^H) \varphi_\ell(-tT_k) \beta \mathbf{e}_1 - V_k \varphi_{\ell-1}(-tT_k) \beta \mathbf{e}_1 + \frac{1}{(\ell-1)!} V_k \beta \mathbf{e}_1 \\ &= t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k - t h_{k+1,k} [\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1] \mathbf{v}_{k+1} \\ &= V_{k+1} \begin{bmatrix} t\gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \\ -t h_{k+1,k} \end{bmatrix} [\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1], \end{aligned}$$

and the relation (3.19) is from (3.18) and (3.1). □

Remark 3.1. Proposition 3.1 indicates that the residual vector $\widehat{\mathbf{r}}_{\ell,k}(t)$ with $\ell \geq 1$ is orthogonal to the space $\text{span}\{(I + \gamma A)V_k\}$, i.e.,

$$\begin{cases} \widehat{\mathbf{y}}_{\ell,k}(t) = V_k \varphi_{\ell}(-tT_k) \beta \mathbf{e}_1 \in \text{span}\{V_k\}, \\ -A\widehat{\mathbf{y}}_{\ell,k}(t) - \frac{\ell}{t}\widehat{\mathbf{y}}_{\ell,k}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \widehat{\mathbf{y}}'_{\ell,k}(t) \perp \text{span}\{(I + \gamma A)V_k\}. \end{cases} \quad (3.20)$$

From (3.7) and (3.20), the residual vectors $\widehat{\mathbf{r}}_{\ell,k}(t)$ ($\ell \geq 0$) are colinear with the residual of the harmonic Ritz pairs [50, 59].

The following theorem establishes the relationship between the Arnoldi method and the harmonic Arnoldi method for φ_{ℓ} functions with $\ell \geq 1$.

Theorem 3.2. Let $\mathbf{y}_{\ell,k}(t) = V_k \varphi_{\ell}(-tH_k) \beta \mathbf{e}_1$ and $\widehat{\mathbf{y}}_{\ell,k}(t) = V_k \varphi_{\ell}(-tT_k) \beta \mathbf{e}_1$ be the approximate solutions obtained from the Arnoldi method and the harmonic Arnoldi method for the φ_{ℓ} ($\ell \geq 1$) functions, respectively; and denote by $\mathbf{r}_{\ell,k}(t)$ and $\widehat{\mathbf{r}}_{\ell,k}(t)$ the corresponding residuals defined in (2.10) and (3.16). If H_k is nonsingular and $k \geq 2$, then we have that

$$\begin{aligned} \widehat{\mathbf{y}}_{\ell,k}(t) - \mathbf{y}_{\ell,k}(t) &= V_k \left[(-tH_k)^{-\ell} \beta \sum_{m=2}^{\infty} \frac{(-t)^m}{m!} \sum_{p=1}^{m-1} [\mathbf{e}_k^H(T_k)^p \mathbf{e}_1] [(H_k)^{m-1-p} \mathbf{g}] \right. \\ &\quad \left. - \sum_{j=1}^{\ell} [\mathbf{e}_k^H \varphi_j(-tT_k) \beta \mathbf{e}_1] (-tH_k)^{-\ell+j} [(H_k)^{-1} \mathbf{g}] \right], \end{aligned} \quad (3.21)$$

and

$$\widehat{\mathbf{r}}_{\ell,k}(t) = \mathbf{r}_{\ell,k}(t) - (h_{k+1,k} \varrho) \mathbf{v}_{k+1} + \gamma h_{k+1,k}^2 [\mathbf{e}_k^H \varphi_{\ell}(-tH_k) \beta \mathbf{e}_1 + \varrho] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k, \quad (3.22)$$

where

$$\varrho = \frac{\beta}{(\ell-1)!} \int_0^1 \sum_{m=2}^{\infty} \left[\frac{t^m (\theta-1)^m}{m!} \right] \sum_{p=1}^{m-1} [\mathbf{e}_k^H(T_k)^p \mathbf{e}_1] [\mathbf{e}_k^H(H_k)^{m-1-p} \mathbf{g}] \theta^{\ell-1} d\theta.$$

Proof. It follows from the recurrence relation of the φ -functions that

$$\varphi_{\ell-1}(-tT_k) \beta \mathbf{e}_1 = -tT_k \varphi_{\ell}(-tT_k) \beta \mathbf{e}_1 + \frac{1}{(\ell-1)!} \beta \mathbf{e}_1, \quad \ell = 1, 2, \dots$$

and

$$\varphi_{\ell-1}(-tH_k) \beta \mathbf{e}_1 = -tH_k \varphi_{\ell}(-tH_k) \beta \mathbf{e}_1 + \frac{1}{(\ell-1)!} \beta \mathbf{e}_1, \quad \ell = 1, 2, \dots$$

Therefore,

$$\varphi_{\ell}(-tT_k) \beta \mathbf{e}_1 - \varphi_{\ell}(-tH_k) \beta \mathbf{e}_1 = (-tH_k)^{-1} \left[\varphi_{\ell-1}(-tT_k) \beta \mathbf{e}_1 - \varphi_{\ell-1}(-tH_k) \beta \mathbf{e}_1 \right] - [(H_k)^{-1} \mathbf{g}] [\mathbf{e}_k^H \varphi_{\ell}(-tT_k) \beta \mathbf{e}_1]. \quad (3.23)$$

Using the same trick, we obtain

$$\begin{aligned} \varphi_{\ell-1}(-tT_k) \beta \mathbf{e}_1 - \varphi_{\ell-1}(-tH_k) \beta \mathbf{e}_1 &= (-tH_k)^{-1} \left[\varphi_{\ell-2}(-tT_k) \beta \mathbf{e}_1 - \varphi_{\ell-2}(-tH_k) \beta \mathbf{e}_1 \right] \\ &\quad - [(H_k)^{-1} \mathbf{g}] [\mathbf{e}_k^H \varphi_{\ell-1}(-tT_k) \beta \mathbf{e}_1]. \end{aligned}$$

As a result, the relation (3.23) can be written as

$$\begin{aligned}
\varphi_\ell(-tT_k)\beta\mathbf{e}_1 - \varphi_\ell(-tH_k)\beta\mathbf{e}_1 &= (-tH_k)^{-1} \left[(-tH_k)^{-1} \left[\varphi_{\ell-2}(-tT_k)\beta\mathbf{e}_1 - \varphi_{\ell-2}(-tH_k)\beta\mathbf{e}_1 \right] \right. \\
&\quad \left. - [(H_k)^{-1}\mathbf{g}] [\mathbf{e}_k^H \varphi_{\ell-1}(-tT_k)\beta\mathbf{e}_1] \right] - [(H_k)^{-1}\mathbf{g}] [\mathbf{e}_k^H \varphi_\ell(-tT_k)\beta\mathbf{e}_1] \\
&= (-tH_k)^{-2} \left[\varphi_{\ell-2}(-tT_k)\beta\mathbf{e}_1 - \varphi_{\ell-2}(-tH_k)\beta\mathbf{e}_1 \right] \\
&\quad - (-tH_k)^{-1} [(H_k)^{-1}\mathbf{g}] [\mathbf{e}_k^H \varphi_{\ell-1}(-tT_k)\beta\mathbf{e}_1] - [(H_k)^{-1}\mathbf{g}] [\mathbf{e}_k^H \varphi_\ell(-tT_k)\beta\mathbf{e}_1].
\end{aligned}$$

By induction,

$$\begin{aligned}
\varphi_\ell(-tT_k)\beta\mathbf{e}_1 - \varphi_\ell(-tH_k)\beta\mathbf{e}_1 &= (-tH_k)^{-\ell} \left[\varphi_0(-tT_k)\beta\mathbf{e}_1 - \varphi_0(-tH_k)\beta\mathbf{e}_1 \right] \\
&\quad - \sum_{j=1}^{\ell} [\mathbf{e}_k^H \varphi_j(-tT_k)\beta\mathbf{e}_1] (-tH_k)^{-\ell+j} [(H_k)^{-1}\mathbf{g}].
\end{aligned}$$

From (3.12), we obtain

$$\begin{aligned}
\varphi_\ell(-tT_k)\beta\mathbf{e}_1 - \varphi_\ell(-tH_k)\beta\mathbf{e}_1 &= (-tH_k)^{-\ell} \beta \sum_{m=2}^{\infty} \frac{(-t)^m}{m!} \sum_{p=1}^{m-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{m-1-p} \mathbf{g}] \\
&\quad - \sum_{j=1}^{\ell} [\mathbf{e}_k^H \varphi_j(-tT_k)\beta\mathbf{e}_1] (-tH_k)^{-\ell+j} [(H_k)^{-1}\mathbf{g}]. \tag{3.24}
\end{aligned}$$

So we get

$$\begin{aligned}
\hat{\mathbf{y}}_{\ell,k}(t) - \mathbf{y}_{\ell,k}(t) &= V_k [\varphi_\ell(-tT_k)\beta\mathbf{e}_1 - \varphi_\ell(-tH_k)\beta\mathbf{e}_1] \\
&= V_k \cdot \left[(-tH_k)^{-\ell} \beta \sum_{m=2}^{\infty} \frac{(-t)^m}{m!} \sum_{p=1}^{m-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [(H_k)^{m-1-p} \mathbf{g}] \right. \\
&\quad \left. - \sum_{j=1}^{\ell} [\mathbf{e}_k^H \varphi_j(-tT_k)\beta\mathbf{e}_1] (-tH_k)^{-\ell+j} [(H_k)^{-1}\mathbf{g}] \right]. \tag{3.25}
\end{aligned}$$

On the other hand, we have that

$$\begin{aligned}
\varphi_\ell(-tT_k)\beta\mathbf{e}_1 &= \frac{1}{(\ell-1)!} \int_0^1 \exp[(1-\theta)(-tT_k)] \theta^{\ell-1} \beta\mathbf{e}_1 d\theta, \\
\varphi_\ell(-tH_k)\beta\mathbf{e}_1 &= \frac{1}{(\ell-1)!} \int_0^1 \exp[(1-\theta)(-tH_k)] \theta^{\ell-1} \beta\mathbf{e}_1 d\theta,
\end{aligned}$$

and we have from (3.12) that

$$\begin{aligned}
\varrho &= \mathbf{e}_k^H \varphi_\ell(-tT_k)\beta\mathbf{e}_1 - \mathbf{e}_k^H \varphi_\ell(-tH_k)\beta\mathbf{e}_1 \\
&= \frac{\beta}{(\ell-1)!} \int_0^1 \sum_{m=2}^{\infty} \left[\frac{t^m (\theta-1)^m}{m!} \right] \sum_{p=1}^{m-1} [\mathbf{e}_k^H (T_k)^p \mathbf{e}_1] [\mathbf{e}_k^H (H_k)^{m-1-p} \mathbf{g}] \theta^{\ell-1} d\theta. \tag{3.26}
\end{aligned}$$

Then we obtain from (3.18) that

$$\begin{aligned}
\hat{\mathbf{r}}_{\ell,k}(t) &= \gamma h_{k+1,k}^2 [\mathbf{e}_k^H \varphi_\ell(-tH_k)\beta\mathbf{e}_1 + \varrho] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k - h_{k+1,k} [\mathbf{e}_k^H \varphi_\ell(-tH_k)\beta\mathbf{e}_1 + \varrho] \mathbf{v}_{k+1} \\
&= \mathbf{r}_{\ell,k}(t) - (h_{k+1,k} \varrho) \mathbf{v}_{k+1} + \gamma h_{k+1,k}^2 [\mathbf{e}_k^H \varphi_\ell(-tH_k)\beta\mathbf{e}_1 + \varrho] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k.
\end{aligned}$$

□

3.3 A thick-restarted harmonic Arnoldi algorithm for φ -functions

When using the Krylov subspace method for approximating the action of a matrix function on a vector, the maximum number of iterations that can be performed is often limited by the storage requirements of the full Arnoldi basis. In this subsection, we propose a thick-restarted harmonic Arnoldi algorithm for the φ -functions. The thick-restarting strategy was firstly proposed by Wu and Simon for large symmetric eigenvalue problem [65], and was generalized to solving large non-Hermitian eigenproblems [35, 45] and linear systems [46].

Our thick-restarted harmonic Arnoldi algorithm is a little similar to the deflated GMRES algorithm for linear systems [46]. So it is simple to implement compared with the deflated Krylov subspace methods proposed in [15, 18]. The key to our new algorithm is two-fold. First, we apply an additive correction to the *residual* of the φ -functions when restarting, instead of the *error* used in [1, 2, 14, 15, 19, 34, 60]. Second, we use the fact that the residual of the harmonic Arnoldi approximation is colinear with that of the harmonic Ritz pairs. Consequently, one can compute the approximations to (1.3) simultaneously in the same search subspace.

Let's consider how to thick-restart the harmonic Arnoldi method for the φ -functions. We denote $\hat{\mathbf{y}}_{0,k}(t) = \hat{\mathbf{y}}_k(t)$ and $\hat{\mathbf{r}}_{0,k}(t) = \hat{\mathbf{r}}_k(t)$. In the first cycle of the thick-restarted harmonic Arnoldi algorithm, we run the k -step Arnoldi process and generate the Arnoldi relation (2.1). We then compute the approximations $\hat{\mathbf{y}}_{0,k}(t)$ and $\hat{\mathbf{y}}_{\ell,k}(t)$ via (3.5) and (3.15), respectively. If the residual norms are larger than a given tolerance tol (see (3.6) and (3.18)), one computes some harmonic Ritz pairs $(\tilde{\lambda}_i, \tilde{\mathbf{x}}_i)$ ($i = 1, 2, \dots, q$) of A , which satisfy [50, 59]

$$\begin{cases} \tilde{\mathbf{x}}_i \in \text{span}\{V_k^{(1)}\}, \\ A\tilde{\mathbf{x}}_i - \tilde{\lambda}_i\tilde{\mathbf{x}}_i \perp (I + \gamma A)\text{span}\{V_k^{(1)}\}. \end{cases} \quad (3.27)$$

For simplicity, we denote by the variables computed from the “previous” cycle with a superscript $(\cdot)^{(1)}$. For instance, $V_k^{(1)}$ represents the orthonormal basis obtained from the “previous” Arnoldi iteration. Let $\tilde{\mathbf{x}}_i = V_k^{(1)}\tilde{\psi}_i$, $i = 1, 2, \dots, q$. We then construct a real matrix using $\{\tilde{\psi}_i\}_{i=1}^q$: separate $\tilde{\psi}_i$ into the real and imaginary part if it is complex, and both parts should be included and adjust q if necessary. Then orthonormalize these vectors in order to form a $k \times q$ orthonormal matrix W_q .

We consider how to establish an Arnoldi-like relation for the new cycle, using the eigen-information retained from the “previous” cycle. Let $\hat{\mathbf{r}}_{\ell,k}^{(1)}(t) = V_{k+1}^{(1)}\mathbf{w}_k^{(1)}(t) \cdot [\mathbf{e}_k^H \varphi_\ell(-tT_k)\beta \mathbf{e}_1]$, where

$$\mathbf{w}_k^{(1)}(t) = \begin{bmatrix} \gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k \\ -h_{k+1,k} \end{bmatrix}. \quad (3.28)$$

Thus, the residuals $\hat{\mathbf{r}}_{\ell,k}^{(1)}(t)$ ($\ell \geq 0$) are colinear with each other and are independent of ℓ . Denote by $\widehat{W}_q = [W_q; \mathbf{0}] \in \mathbb{R}^{(k+1) \times q}$ the matrix obtained from appending a zero row at the bottom of W_q , then

$$\begin{aligned} AV_k^{(1)}W_q &\subseteq \text{span}\{V_k^{(1)}W_q, \hat{\mathbf{r}}_{\ell,k}^{(1)}(t)\} \\ &= \text{span}\left\{V_{k+1}^{(1)}[\widehat{W}_q, \mathbf{w}_k^{(1)}(t)/\|\mathbf{w}_k^{(1)}(t)\|_2]\right\} \\ &= \text{span}\{V_{k+1}^{(1)}W_{q+1}\}, \end{aligned} \quad (3.29)$$

where $W_{q+1} = [\widehat{W}_q, \mathbf{w}_k^{(1)}(t)/\|\mathbf{w}_k^{(1)}(t)\|_2] \in \mathbb{R}^{(k+1) \times (q+1)}$. We orthonormalize the columns of W_{q+1} and still denote the resulting $(k+1)$ -by- $(q+1)$ matrix by W_{q+1} . Let $V_q^{new} = V_k^{(1)}W_q$ and $V_{q+1}^{new} = V_{k+1}^{(1)}W_{q+1}$, by (3.29), there is a $(q+1) \times q$ matrix \bar{H}_q^{new} such that

$$AV_k^{(1)}W_q = AV_q^{new} = (V_{k+1}^{(1)}W_{q+1})\bar{H}_q^{new} = V_{q+1}^{new}\bar{H}_q^{new},$$

where $\bar{H}_q^{new} = (V_{q+1}^{new})^H AV_q^{new}$. Then we have the following relation

$$AV_q^{new} = V_{q+1}^{new} \bar{H}_q^{new}.$$

We then apply the standard Arnoldi process by using $\mathbf{v}_{q+1}^{new} = V_{q+1}^{new}(:, q+1)$ (i.e., the $(q+1)$ -th column of V_{q+1}^{new}) as the initial vector, to form the orthonormal basis $V_{k+1}^{(2)}$ for the new cycle

$$AV_k^{(2)} = V_k^{(2)} H_k^{(2)} + h_{k+1,k}^{(2)} \mathbf{v}_{k+1}^{(2)} \mathbf{e}_k^H = V_{k+1}^{(2)} \bar{H}_k^{(2)}. \quad (3.30)$$

Therefore, some recurrences similar to the Arnoldi recurrence (2.1) are generated by the thick-restarted Arnoldi algorithm. Notice that the matrix composed of the first $(q+1)$ rows and the first q columns of $H_k^{(2)}$ is full rather than upper Hessenberg. Furthermore, one only requires to perform $(k-q)$ matrix-vector products at each cycle after the first, since the first q matrix-vector products are carried out “implicitly”.

We discuss how to update the approximate solution in the new search space $\text{span}\{V_k^{(2)}\}$. We first consider how to update the approximation $\hat{\mathbf{y}}_{0,k}^{(2)}(t)$ for the matrix exponential. To do this, we seek a vector $\hat{\mathbf{z}}_{0,k}^{(2)}(t)$ such that

$$\hat{\mathbf{y}}_{0,k}^{(2)}(t) = \hat{\mathbf{y}}_{0,k}^{(1)}(t) + V_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) \quad (3.31)$$

is a new approximation to $\mathbf{y}(t)$. We note that

$$\begin{aligned} \hat{\mathbf{r}}_{0,k}^{(2)}(t) &= -A\hat{\mathbf{y}}_{0,k}^{(2)}(t) - \hat{\mathbf{y}}_{0,k}^{(2)}(t)' \\ &= -A[V_k^{(1)} \hat{\mathbf{u}}_{0,k}^{(1)}(t) + V_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t)] - [V_k^{(1)} \hat{\mathbf{u}}_{0,k}^{(1)}(t)' + V_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t)'] \\ &= [-AV_k^{(1)} \hat{\mathbf{u}}_{0,k}^{(1)}(t) - V_k^{(1)} \hat{\mathbf{u}}_{0,k}^{(1)}(t)'] - AV_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) - V_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t)' \\ &= \hat{\mathbf{r}}_{0,k}^{(1)}(t) - AV_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) - V_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t)'. \end{aligned} \quad (3.32)$$

Recall from the thick-restarting procedure that $\hat{\mathbf{r}}_{0,k}^{(1)}(t) \in \text{span}\{V_{k+1}^{(2)}\}$, so there exists a vector $\mathbf{c}_{0,k}^{(2)}(t)$ such that $\hat{\mathbf{r}}_{0,k}^{(1)}(t) = V_{k+1}^{(2)} \mathbf{c}_{0,k}^{(2)}(t)$. Let

$$\hat{\mathbf{r}}_{0,k}^{(2)}(t) \perp \text{span}\{(I + \gamma A)V_k^{(2)}\},$$

that is,

$$[(I + \gamma A)V_k^{(2)}]^H [V_{k+1}^{(2)} \mathbf{c}_{0,k}^{(2)}(t) - AV_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) - V_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t)'] = \mathbf{0},$$

we obtain

$$\begin{cases} \hat{\mathbf{z}}_{0,k}^{(2)}(t)' = -\Xi_k^{(2)} \bar{H}_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) + \Xi_k^{(2)} \mathbf{c}_{0,k}^{(2)}(t), \\ \hat{\mathbf{z}}_{0,k}^{(2)}(0) = \mathbf{0}, \end{cases} \quad (3.33)$$

where

$$\Xi_k^{(2)} = (I + \gamma H_k^{(2)})^{-H} (\bar{I} + \gamma \bar{H}_k^{(2)})^H, \quad (3.34)$$

and \bar{I} is the $(k+1) \times k$ matrix being the $k \times k$ identity matrix with an additional zero row at the bottom.

Thus, we update the approximate solution to $\mathbf{y}(t)$ via solving a small-sized ODE (3.33). The residual is

$$\begin{aligned} \hat{\mathbf{r}}_{0,k}^{(2)}(t) &= V_{k+1}^{(2)} \mathbf{c}_{0,k}^{(2)}(t) - V_{k+1}^{(2)} \bar{H}_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) - V_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t)' \\ &= V_{k+1}^{(2)} \left[\mathbf{c}_{0,k}^{(2)}(t) - \bar{H}_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) - \begin{bmatrix} \hat{\mathbf{z}}_{0,k}^{(2)}(t)' \\ 0 \end{bmatrix} \right], \end{aligned} \quad (3.35)$$

with

$$\|\hat{\mathbf{r}}_{0,k}^{(2)}(t)\|_2 = \left\| \mathbf{c}_{0,k}^{(2)}(t) - \bar{H}_k^{(2)} \hat{\mathbf{z}}_{0,k}^{(2)}(t) - \begin{bmatrix} \hat{\mathbf{z}}_{0,k}^{(2)}(t)' \\ 0 \end{bmatrix} \right\|_2. \quad (3.36)$$

Next we discuss how to update the approximate solution for the φ_ℓ ($\ell \geq 1$) functions during cycles. Similarly, given the new search subspace $V_k^{(2)}$ and the approximation $\hat{\mathbf{y}}_{\ell,k}^{(1)}(t)$ obtained from the “previous” cycle, we seek a vector $\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)$ such that

$$\hat{\mathbf{y}}_{\ell,k}^{(2)}(t) = \hat{\mathbf{y}}_{\ell,k}^{(1)}(t) + V_k^{(2)} \hat{\mathbf{z}}_{\ell,k}^{(2)}(t) \quad (3.37)$$

is the new approximation to $\mathbf{y}(t)$. The residual is

$$\begin{aligned} \hat{\mathbf{r}}_{\ell,k}^{(2)}(t) &= -A\hat{\mathbf{y}}_{\ell,k}^{(2)}(t) - \frac{\ell}{t}\hat{\mathbf{y}}_{\ell,k}^{(2)}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \hat{\mathbf{y}}_{\ell,k}^{(2)}(t)' \\ &= -A\left[\hat{\mathbf{y}}_{\ell,k}^{(1)}(t) + V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)\right] - \frac{\ell}{t}\left[\hat{\mathbf{y}}_{\ell,k}^{(1)}(t) + V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)\right] + \frac{1}{t(\ell-1)!}\mathbf{v} - \left[\hat{\mathbf{y}}_{\ell,k}^{(1)}(t)' + V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)'\right] \\ &= \left[-A\hat{\mathbf{y}}_{\ell,k}^{(1)}(t) - \frac{\ell}{t}\hat{\mathbf{y}}_{\ell,k}^{(1)}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \hat{\mathbf{y}}_{\ell,k}^{(1)}(t)'\right] \\ &\quad - AV_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - \frac{\ell}{t}V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)'. \end{aligned} \quad (3.38)$$

It follows from the thick-restarting strategy that

$$\hat{\mathbf{r}}_{\ell,k}^{(1)}(t) = -A\hat{\mathbf{y}}_{\ell,k}^{(1)}(t) - \frac{\ell}{t}\hat{\mathbf{y}}_{\ell,k}^{(1)}(t) + \frac{1}{t(\ell-1)!}\mathbf{v} - \hat{\mathbf{y}}_{\ell,k}^{(1)}(t)' \in \text{span}\{V_{k+1}^{(2)}\}.$$

So there exists a vector $\mathbf{c}_{\ell,k}^{(2)}(t)$ such that $\hat{\mathbf{r}}_{\ell,k}^{(1)}(t) = V_{k+1}^{(2)}\mathbf{c}_{\ell,k}^{(2)}(t)$. Let

$$\hat{\mathbf{r}}_{\ell,k}^{(2)}(t) = V_{k+1}^{(2)}\mathbf{c}_{\ell,k}^{(2)}(t) - AV_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - \frac{\ell}{t}V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)' \perp \text{span}\{(I + \gamma A)V_k^{(2)}\},$$

i.e.,

$$[(I + \gamma A)V_k^{(2)}]^\text{H} \left[V_{k+1}^{(2)}\mathbf{c}_{\ell,k}^{(2)}(t) - AV_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - \frac{\ell}{t}V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)' \right] = \mathbf{0},$$

then

$$\begin{cases} \hat{\mathbf{z}}_{\ell,k}^{(2)}(t)' = -[\Xi_k^{(2)}\bar{H}_k^{(2)} + \frac{\ell}{t}I]\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) + \Xi_k^{(2)}\mathbf{c}_{\ell,k}^{(2)}(t), \\ \hat{\mathbf{z}}_{\ell,k}^{(2)}(0) = \mathbf{0}, \end{cases} \quad (3.39)$$

where $\Xi_k^{(2)}$ is defined in (3.34). Therefore, we update (3.37) by solving the above small-sized ODE. The residual is

$$\begin{aligned} \hat{\mathbf{r}}_{\ell,k}^{(2)}(t) &= V_{k+1}^{(2)}\mathbf{c}_{\ell,k}^{(2)}(t) - V_{k+1}^{(2)}\bar{H}_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - \frac{\ell}{t}V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - V_k^{(2)}\hat{\mathbf{z}}_{\ell,k}^{(2)}(t)' \\ &= V_{k+1}^{(2)}\left[\mathbf{c}_{\ell,k}^{(2)}(t) - (\bar{H}_k^{(2)} + \frac{\ell}{t}I)\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - \begin{bmatrix} \hat{\mathbf{z}}_{\ell,k}^{(2)}(t)' \\ 0 \end{bmatrix}\right], \quad \ell \geq 1, \end{aligned} \quad (3.40)$$

and

$$\|\hat{\mathbf{r}}_{\ell,k}^{(2)}(t)\|_2 = \left\| \mathbf{c}_{\ell,k}^{(2)}(t) - [\bar{H}_k^{(2)} + \frac{\ell}{t}I]\hat{\mathbf{z}}_{\ell,k}^{(2)}(t) - \begin{bmatrix} \hat{\mathbf{z}}_{\ell,k}^{(2)}(t)' \\ 0 \end{bmatrix} \right\|_2, \quad \ell \geq 1. \quad (3.41)$$

When $\ell = 0$, it is seen that (3.39) and (3.40) reduce to (3.33) and (3.35), respectively.

In summary, we propose the main algorithm of this paper for solving (1.3).

Algorithm 1. A thick-restarted harmonic Arnoldi algorithm for the action of φ -functions on a vector (TRHA)

Step 1. Given the matrix A , the vector \mathbf{v} , the values of t and s , a shift γ , as well as a convergence tolerance tol . Specify k , the steps of the Arnoldi process, and q , the number of approximate eigenvectors which are retained from one cycle to the next;

Step 2. Run the k -step Arnoldi process to form V_{k+1} and H_k . Compute the approximate solutions $\hat{\mathbf{y}}_{\ell,k}(t)$ ($\ell = 0, 1, \dots, s$). If all the residual norms are below tol (see (3.6) and (3.18)), then stop, else compute the primitive harmonic Ritz pairs $(\tilde{\lambda}_i, \tilde{\psi}_i)$, $i = 1, 2, \dots, k$, and select q of them. Go to **Step 4**;

Step 3. Run the remaining $(k - q)$ steps of Arnoldi process to form V_{k+1} and H_k , using the last column of V_{q+1} as the initial vector. Update the approximation $\hat{\mathbf{y}}_{\ell,k}(t)$ by solving (3.39) ($\ell = 0, 1, \dots, s$), if all the residual norms are below tol (see (3.41)), then stop, otherwise compute primitive Ritz pairs $(\tilde{\lambda}_i, \tilde{\psi}_i)$, $i = 1, 2, \dots, k$, and select q of them;

Step 4. Orthonormalize the $\{\tilde{\psi}_i\}'s$, $i = 1, 2, \dots, q$, to form a real k -by- q matrix $W_q = [\tilde{\psi}_1, \tilde{\psi}_2, \dots, \tilde{\psi}_q]$. If $\tilde{\psi}_i$ is complex, separate it into the real part and the imaginary part, both parts should be included, and adjust q if necessary (increasing or decreasing q by 1);

Step 5. Extend W_q to a $(k + 1) \times q$ matrix $\hat{W}_q = [W_q; \mathbf{0}]$, where $\mathbf{0}$ is a zero row vector. Let $W_{q+1} = [\hat{W}_q, \mathbf{w}_k(t)/\|\mathbf{w}_k(t)\|_2]$. Then orthonormalize the columns of W_{q+1} to yield an orthonormal matrix with size $(k + 1) \times (q + 1)$;

Step 6. Form the portions of new \bar{H}_k and V_{k+1} by using the old \bar{H}_k and V_{k+1} : Let $\bar{H}_q^{\text{new}} = W_{q+1}^H \bar{H}_k W_q$ and $V_{q+1}^{\text{new}} = V_{k+1} W_{q+1}$, then set $\bar{H}_q = \bar{H}_q^{\text{new}}$ and $V_{q+1} = V_{q+1}^{\text{new}}$. Go to **Step 3**.

Remark 3.2. Two remarks are in order. First, since the residuals $\hat{\mathbf{r}}_{\ell,k}(t)$ ($\ell = 0, 1, 2, \dots, s$) are colinear with each other, one can solve the vectors $\varphi_{\ell}(-tA)\mathbf{v}$ ($\ell = 0, 1, \dots, s$) simultaneously, and compute them in the same search subspace. Second, as a by-product, we can also present a thick-restarted Arnoldi algorithm for the φ -functions. The difference is that one evaluates the Arnoldi approximations $\mathbf{y}_{\ell,k}(t)$ via the orthogonal projection technique (2.3) and (2.18), and augments the search subspace with the Ritz vectors rather than harmonic Ritz vectors.

4 Relationship between the error and the residual of the approximations

In this section, we investigate the relationship between the error and the residual of the (harmonic) Arnoldi approximation for φ -functions. Let Γ be a closed contour that encloses the spectra of $-tA$ and $-tH_k$. Let $\mathbf{y}(t) = \varphi_{\ell}(-tA)\mathbf{v}$ and let $\mathbf{y}_{\ell,k}(t) = V_k \varphi_{\ell}(-tH_k) \beta \mathbf{e}_1$ be the approximation from the Arnoldi method, where $\mathbf{y}_{0,k}(t) \equiv \mathbf{y}_k(t)$ is the Arnoldi approximation for matrix exponential. If φ_{ℓ} ($\ell \geq 0$) are analytic on and inside the closed contour Γ , from the Dunford-Taylor integral representation [27], we obtain

$$\mathbf{y}(t) = \varphi_{\ell}(-tA)\mathbf{v} = \frac{1}{2\pi i} \int_{\Gamma} \varphi_{\ell}(z)(zI + tA)^{-1} \mathbf{v} dz, \quad \ell = 0, 1, 2, \dots \quad (4.1)$$

where $i^2 = -1$. Moreover,

$$\mathbf{y}_{\ell,k}(t) = V_k \varphi_{\ell}(-tH_k) \beta \mathbf{e}_1 = \frac{1}{2\pi i} \int_{\Gamma} \varphi_{\ell}(z) V_k (zI + tH_k)^{-1} \beta \mathbf{e}_1 dz, \quad \ell = 0, 1, 2, \dots \quad (4.2)$$

We have the following theorem on the Arnoldi approximation for φ -functions.

Theorem 4.1. Denote by $\mathbf{e}_{\ell,k}(t) = \mathbf{y}(t) - \mathbf{y}_{\ell,k}(t)$ the error, and by $\mathbf{r}_{\ell,k}(t)$ the residual with respect to $\mathbf{y}_{\ell,k}(t)$, where $\mathbf{r}_{0,k}(t) \equiv \mathbf{r}_k(t)$ is the residual of the Arnoldi approximation to matrix exponential. Assume that $\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1 \neq 0$, and denote

$$f_{H_k}(z) = t\varphi_\ell(z) \cdot \frac{\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1}.$$

Then we have

$$\mathbf{e}_{\ell,k}(t) = \frac{1}{2\pi i} \int_{\Gamma} f_{H_k}(z) (zI + tA)^{-1} \cdot \mathbf{r}_{\ell,k}(t) dz,$$

and

$$\|\mathbf{e}_{\ell,k}(t)\|_2 \leq \left\| \frac{1}{2\pi i} \int_{\Gamma} f_{H_k}(z) (zI + tA)^{-1} dz \right\|_2 \cdot \|\mathbf{r}_{\ell,k}(t)\|_2. \quad (4.3)$$

Proof. It follows that

$$\begin{aligned} \mathbf{e}_{\ell,k}(t) &= \mathbf{y}(t) - \mathbf{y}_{\ell,k}(t) \\ &= \frac{1}{2\pi i} \int_{\Gamma} \varphi_\ell(z) [(zI + tA)^{-1} \mathbf{v} - V_k(zI + tH_k)^{-1} \beta \mathbf{e}_1] dz, \end{aligned}$$

and

$$(zI + tA)^{-1} \mathbf{v} - V_k(zI + tH_k)^{-1} \beta \mathbf{e}_1 = (zI + tA)^{-1} [\mathbf{v} - (zI + tA)V_k(zI + tH_k)^{-1} \beta \mathbf{e}_1].$$

From the Arnoldi relation (2.1), we get

$$\mathbf{v} - (zI + tA)V_k(zI + tH_k)^{-1} \beta \mathbf{e}_1 = -th_{k+1,k} [\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1}.$$

Recall that $\mathbf{r}_{\ell,k}(t) = -h_{k+1,k} [\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1] \mathbf{v}_{k+1}$, thus

$$\begin{aligned} \mathbf{e}_{\ell,k}(t) &= \frac{1}{2\pi i} \int_{\Gamma} \varphi_\ell(z) (zI + tA)^{-1} [-th_{k+1,k} [\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1}] dz \\ &= \frac{1}{2\pi i} \int_{\Gamma} \varphi_\ell(z) (zI + tA)^{-1} \frac{\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1} [-th_{k+1,k} [\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1] \mathbf{v}_{k+1}] dz \\ &= \frac{1}{2\pi i} \int_{\Gamma} t\varphi_\ell(z) \frac{\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1} \cdot (zI + tA)^{-1} \mathbf{r}_{\ell,k}(t) dz. \end{aligned} \quad (4.4)$$

Let $f_{H_k}(z) = t\varphi_\ell(z) \frac{\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1}$, and notice that

$$\frac{1}{2\pi i} \int_{\Gamma} t\varphi_\ell(z) \frac{\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1} dz = \frac{1}{2\pi i} \int_{\Gamma} f_{H_k}(z) dz = t. \quad (4.5)$$

Therefore, we have from (4.4) that

$$\begin{aligned} \|\mathbf{e}_{\ell,k}(t)\|_2 &= \left\| \frac{1}{2\pi i} \int_{\Gamma} f_{H_k}(z) (zI + tA)^{-1} dz \cdot \mathbf{r}_{\ell,k}(t) \right\|_2 \\ &\leq \left\| \frac{1}{2\pi i} \int_{\Gamma} f_{H_k}(z) (zI + tA)^{-1} dz \right\|_2 \cdot \|\mathbf{r}_{\ell,k}(t)\|_2. \end{aligned}$$

□

Now we focus on error estimates of a class of special matrices. Denote the numerical range of A by $W(A)$, i.e.,

$$W(A) = \left\{ \frac{(A\mathbf{x}, \mathbf{x})}{(\mathbf{x}, \mathbf{x})}, \mathbf{0} \neq \mathbf{x} \in \mathbb{C}^n \right\},$$

where (\cdot, \cdot) represents the Euclidean inner product. Note that $W(H_k) \subseteq W(A)$ holds for each k . For $a \geq 0$ and $0 \leq \vartheta \leq \pi/2$, we define the set

$$\Sigma_{\vartheta, a} = \{z \in \mathbb{C} : |\arg(z - a)| \leq \vartheta\},$$

where $\arg(\cdot)$ denotes the argument of a complex number; and assume that

$$W(A) \subset \Sigma_{\vartheta, a}. \quad (4.6)$$

It is known that this assumption holds in important applications such as parabolic partial differential equations.

Similar to [12], our analysis is based on the integral representation [12, 16]

$$\mathbf{y}(t) = \frac{1}{t^\ell} \lim_{N \rightarrow \infty} \frac{1}{2\pi \mathbf{i}} \int_{\varepsilon - \mathbf{i}N}^{\varepsilon + \mathbf{i}N} \frac{\exp(tz)}{z^\ell} (zI + A)^{-1} \mathbf{v} dz, \quad \ell = 0, 1, 2, \dots,$$

which, under our assumptions, holds for every $\varepsilon > 0$ with uniform convergence when t is chosen in compact intervals of $(0, +\infty)$. Given $\varepsilon > 0$, if we set $z = \varepsilon + \mathbf{i}\rho$, then [12]

$$\mathbf{y}(t) = \frac{\exp(t\varepsilon)}{t^\ell} \lim_{N \rightarrow \infty} \frac{1}{2\pi} \int_{-N}^{+N} \frac{\exp(\mathbf{i}t\rho)}{(\varepsilon + \mathbf{i}\rho)^\ell} ((\varepsilon + \mathbf{i}\rho)I + A)^{-1} \mathbf{v} d\rho.$$

Suppose that $A \in \mathbb{R}^{n \times n}$ is a real matrix. Consider $\mu_j = a_j + \mathbf{i}b_j$ ($j = 1, 2, \dots, k$) the eigenvalues of matrix H_k arranging as μ_1, \dots, μ_{k_1} the real ones and $\mu_{k_1+1}, \dots, \mu_k$ the complex conjugate ones. Let

$$r_j = ((\varepsilon + a_j)^2 + b_j^2)^{1/2}, \quad R = \max_{1 \leq j \leq k} r_j,$$

and

$$\omega_k(\varepsilon) = \prod_{j=1}^k (r_j(\varepsilon + a_j))^{1/2}.$$

Define

$$\varsigma_k(\rho) = \prod_{j=1}^{k_1} (1 + \rho^2/r_j^2)^{1/2} \prod_{j=k_1+1}^k (1 + \rho^2/r_j^2)^{1/4},$$

and

$$d_k(\rho) = \frac{\prod_{j=1}^{k-1} h_{j+1,j}}{\omega_k(\varepsilon) \varsigma_k(\rho)}. \quad (4.7)$$

Under the above assumptions, we can prove the following result whose proof is along the line of Proposition 5 of [12].

Theorem 4.2. *Let $\varepsilon > 0$ and suppose $k + k_1 + 2\ell \geq 4$. Then for the Arnoldi approximation, we have*

$$\|\mathbf{e}_{\ell,k}(t)\|_2 \leq c_{\ell,k} \cdot \int_0^\infty \frac{(1 + \rho^2/\varepsilon^2)^{-\ell/2}}{\varsigma_k(\rho)} d\rho \cdot \|\mathbf{r}_{\ell,k}(t)\|_2 \quad (4.8)$$

where $c_{\ell,k} = \frac{\exp(t\varepsilon)}{\pi(t\varepsilon)^\ell \omega_k(\varepsilon)(\varepsilon + a)} \cdot \frac{\prod_{j=1}^{k-1} h_{j+1,j}}{|\mathbf{e}_k^\top \varphi_\ell(-tH_k) \mathbf{e}_1|}$.

Proof. It follows that

$$\begin{aligned}\mathbf{e}_{\ell,k}(t) &= \mathbf{y}(t) - \mathbf{y}_{\ell,k}(t) \\ &= \frac{\exp(t\varepsilon)}{t^\ell} \lim_{N \rightarrow \infty} \frac{1}{2\pi} \int_{-N}^{+N} \frac{\exp(i\rho t)}{(\varepsilon + i\rho)^\ell} \left[((\varepsilon + i\rho)I + A)^{-1} \mathbf{v} - V_k((\varepsilon + i\rho)I + H_k)^{-1} \beta \mathbf{e}_1 \right] d\rho,\end{aligned}$$

and

$$\begin{aligned}& ((\varepsilon + i\rho)I + A)^{-1} \mathbf{v} - V_k((\varepsilon + i\rho)I + H_k)^{-1} \beta \mathbf{e}_1 \\ &= ((\varepsilon + i\rho)I + A)^{-1} \left[\mathbf{v} - ((\varepsilon + i\rho)I + A) V_k((\varepsilon + i\rho)I + H_k)^{-1} \beta \mathbf{e}_1 \right].\end{aligned}$$

From the Arnoldi relation (2.1), we obtain

$$\mathbf{v} - ((\varepsilon + i\rho)I + A) V_k((\varepsilon + i\rho)I + H_k)^{-1} \beta \mathbf{e}_1 = -h_{k+1,k} \left[\mathbf{e}_k^H((\varepsilon + i\rho)I + H_k)^{-1} \beta \mathbf{e}_1 \right] \mathbf{v}_{k+1}.$$

Recall that $\mathbf{r}_{\ell,k}(t) = -h_{k+1,k} [\mathbf{e}_k^H \varphi_\ell(-tH_k) \beta \mathbf{e}_1] \mathbf{v}_{k+1}$, thus

$$\mathbf{e}_{\ell,k}(t) = \frac{\exp(t\varepsilon)}{t^\ell} \lim_{N \rightarrow \infty} \frac{1}{2\pi} \int_{-N}^{+N} \frac{\exp(i\rho t)}{(\varepsilon + i\rho)^\ell} ((\varepsilon + i\rho)I + A)^{-1} \frac{\mathbf{e}_k^H((\varepsilon + i\rho)I + H_k)^{-1} \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tH_k) \mathbf{e}_1} \mathbf{r}_{\ell,k}(t) d\rho. \quad (4.9)$$

It follows from Lemma 2 of [12] that

$$|\mathbf{e}_k^H((\varepsilon + i\rho)I + H_k)^{-1} \mathbf{e}_1| = \left| \det((\varepsilon + i\rho)I + H_k)^{-1} \prod_{j=1}^{k-1} h_{j+1,j} \right|. \quad (4.10)$$

Moreover, we have from Proposition 5 of [12] that

$$|\mathbf{e}_k^H((\varepsilon + i\rho)I + H_k)^{-1} \mathbf{e}_1| \leq d_k(\rho), \quad (4.11)$$

and

$$\|((\varepsilon + i\rho)I + A)^{-1}\|_2 \leq (\varepsilon + a)^{-1}. \quad (4.12)$$

By means of (4.10)–(4.12), we obtain from (4.7) and (4.9) that

$$\begin{aligned}\|\mathbf{e}_{\ell,k}(t)\|_2 &\leq \frac{\exp(t\varepsilon)}{\pi t^\ell (\varepsilon + a)} \cdot \frac{1}{|\mathbf{e}_k^H \varphi_\ell(-tH_k) \mathbf{e}_1|} \cdot \int_0^\infty \frac{d_k(\rho)}{(\varepsilon^2 + \rho^2)^{\ell/2}} d\rho \cdot \|\mathbf{r}_{\ell,k}(t)\|_2 \\ &= c_{\ell,k} \cdot \int_0^\infty \frac{(1 + \rho^2/\varepsilon^2)^{-\ell/2}}{\varsigma_k(\rho)} d\rho \cdot \|\mathbf{r}_{\ell,k}(t)\|_2.\end{aligned}$$

Thus (4.8) is proved. We notice that if $k + k_1 + 2\ell \geq 4$, then the integral in (4.8) converges. \square

The following result avoids the use of a quadrature rule for evaluating the integral in (4.8). The proof is similar to Proposition 6 of [12] and is omitted.

Theorem 4.3. *Let $\varepsilon > 0$ and suppose that $k + k_1 \geq 4$. Under the above notations, we have*

$$\|\mathbf{e}_{\ell,k}(t)\|_2 \leq c_{\ell,k} \cdot C_k \cdot \|\mathbf{r}_{\ell,k}(t)\|_2,$$

where

$$C_k = \frac{\sqrt{\pi}}{2\sqrt{S_1}} + \exp(-\varepsilon^2 S_2)(R - \varepsilon) + \left(\frac{\varepsilon}{\sqrt{\varepsilon^2 + R^2}} \right)^\ell \frac{\pi R}{2^{(\frac{k+k_1}{4}+1)}},$$

with

$$S_1 = \frac{\ell}{4\varepsilon^2} + \frac{1}{2} \sum_{j=1}^{k_1} \frac{1}{r_j^2 + \varepsilon^2} + \frac{1}{4} \sum_{j=k_1+1}^k \frac{1}{r_j^2 + \varepsilon^2},$$

and

$$S_2 = \frac{\ell}{2(\varepsilon^2 + R^2)} + \frac{1}{2} \sum_{j=1}^{k_1} \frac{1}{r_j^2 + R^2} + \frac{1}{4} \sum_{j=k_1+1}^k \frac{1}{r_j^2 + R^2}.$$

Next, we consider the harmonic Arnoldi approximation. Let $\hat{\Gamma}$ be a closed contour that encloses the spectra of $-tA$ and $-tT_k$. Let $\hat{\mathbf{y}}_{\ell,k}(t) = V_k \varphi_\ell(-tT_k) \beta \mathbf{e}_1$ be the approximation from the harmonic Arnoldi method, where $\hat{\mathbf{y}}_{0,k}(t) \equiv \hat{\mathbf{y}}_k(t)$ is the harmonic Arnoldi approximation for matrix exponential. If φ_ℓ ($\ell \geq 0$) are analytic on and inside the closed contour $\hat{\Gamma}$, we obtain from the Dunford-Taylor integral representation that

$$\hat{\mathbf{y}}_{\ell,k}(t) = V_k \varphi_\ell(-tT_k) \beta \mathbf{e}_1 = \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_\ell(z) V_k (zI + tT_k)^{-1} \beta \mathbf{e}_1 dz, \quad \ell = 0, 1, 2, \dots \quad (4.13)$$

We are ready to present the following theorem on the relation between the error and the residual of the harmonic Arnoldi approximation $\hat{\mathbf{y}}_{\ell,k}(t)$.

Theorem 4.4. Denote by $\hat{\mathbf{e}}_{\ell,k}(t) = \mathbf{y}(t) - \hat{\mathbf{y}}_{\ell,k}(t)$ the error, and by $\hat{\mathbf{r}}_{\ell,k}(t)$ the residual with respect to $\hat{\mathbf{y}}_{\ell,k}(t)$, where $\hat{\mathbf{r}}_{0,k}(t) \equiv \hat{\mathbf{r}}_k(t)$ is the residual of the harmonic Arnoldi approximation to matrix exponential. Assume that $\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1 \neq 0$, and define

$$f_{T_k}(z) = t \varphi_\ell(z) \cdot \frac{\mathbf{e}_k^H (zI + tT_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1}.$$

Then we have

$$\hat{\mathbf{e}}_{\ell,k}(t) = \frac{1}{2\pi i} \int_{\hat{\Gamma}} f_{T_k}(z) (zI + tA)^{-1} dz \cdot \hat{\mathbf{r}}_{\ell,k}(t),$$

and

$$\|\hat{\mathbf{e}}_{\ell,k}(t)\|_2 \leq \left\| \frac{1}{2\pi i} \int_{\hat{\Gamma}} f_{T_k}(z) (zI + tA)^{-1} dz \right\|_2 \cdot \|\hat{\mathbf{r}}_{\ell,k}(t)\|_2. \quad (4.14)$$

Proof. From the Dunford-Taylor representation, we have

$$\mathbf{y}(t) = \varphi_\ell(-tA) \mathbf{v} = \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_\ell(z) (zI + tA)^{-1} \mathbf{v} dz, \quad \ell = 0, 1, 2, \dots \quad (4.15)$$

and

$$\hat{\mathbf{y}}_{\ell,k}(t) = V_k \varphi_\ell(-tT_k) \beta \mathbf{e}_1 = \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_\ell(z) V_k (zI + tT_k)^{-1} \beta \mathbf{e}_1 dz, \quad \ell = 0, 1, 2, \dots \quad (4.16)$$

So we have

$$\begin{aligned} \hat{\mathbf{e}}_{\ell,k}(t) &= \mathbf{y}(t) - \hat{\mathbf{y}}_{\ell,k}(t) \\ &= \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_\ell(z) [(zI + tA)^{-1} \mathbf{v} - V_k (zI + tT_k)^{-1} \beta \mathbf{e}_1] dz. \end{aligned}$$

Moreover, by (2.1) and (3.4), we get the following relation

$$\begin{aligned} \mathbf{v} - (zI + tA) V_k (zI + tT_k)^{-1} \beta \mathbf{e}_1 &= t \gamma h_{k+1,k}^2 [\mathbf{e}_k^H (zI + tT_k)^{-1} \beta \mathbf{e}_1] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k \\ &\quad - t h_{k+1,k} [\mathbf{e}_k^H (zI + tT_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1}. \end{aligned}$$

If $\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1 \neq 0$, we obtain from (3.6) and (3.18) that

$$\begin{aligned}
\widehat{\mathbf{e}}_{\ell,k}(t) &= \frac{1}{2\pi\mathbf{i}} \int_{\widehat{\Gamma}} \varphi_\ell(z) (zI + tA)^{-1} \left[t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1] V_k(I + \gamma H_k)^{-H} \mathbf{e}_k \right. \\
&\quad \left. - t h_{k+1,k} [\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1} \right] dz \\
&= \frac{1}{2\pi\mathbf{i}} \int_{\widehat{\Gamma}} \varphi_\ell(z) (zI + tA)^{-1} \frac{\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1} \left[t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1] V_k(I + \gamma H_k)^{-H} \mathbf{e}_k \right. \\
&\quad \left. - t h_{k+1,k} [\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1] \mathbf{v}_{k+1} \right] dz \\
&= \frac{1}{2\pi\mathbf{i}} \int_{\widehat{\Gamma}} t\varphi_\ell(z) \frac{\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1} \cdot (zI + tA)^{-1} \widehat{\mathbf{r}}_{\ell,k}(t) dz.
\end{aligned} \tag{4.17}$$

Let $f_{T_k}(z) = t\varphi_\ell(z) \frac{\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1}$, and notice that

$$\frac{1}{2\pi\mathbf{i}} \int_{\widehat{\Gamma}} t\varphi_\ell(z) \frac{\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1}{\mathbf{e}_k^H \varphi_\ell(-tT_k) \beta \mathbf{e}_1} dz = \frac{1}{2\pi\mathbf{i}} \int_{\widehat{\Gamma}} f_{T_k}(z) dz = t. \tag{4.18}$$

Therefore, we have from (4.17) that

$$\begin{aligned}
\|\widehat{\mathbf{e}}_{\ell,k}(t)\|_2 &= \left\| \frac{1}{2\pi\mathbf{i}} \int_{\widehat{\Gamma}} f_{T_k}(z) (zI + tA)^{-1} dz \cdot \widehat{\mathbf{r}}_{\ell,k}(t) \right\|_2 \\
&\leq \left\| \frac{1}{2\pi\mathbf{i}} \int_{\widehat{\Gamma}} f_{T_k}(z) (zI + tA)^{-1} dz \right\|_2 \cdot \|\widehat{\mathbf{r}}_{\ell,k}(t)\|_2.
\end{aligned}$$

□

Similar to the Arnoldi approximation, we can give an error estimate of a class of special matrices where the assumption (4.6) holds. Let $\widehat{\mu}_j = \widehat{a}_j + \mathbf{i}\widehat{b}_j$ ($j = 1, 2, \dots, k$) be the eigenvalues of matrix T_k arranging as $\widehat{\mu}_1, \dots, \widehat{\mu}_{k_2}$ the real ones and $\widehat{\mu}_{k_2+1}, \dots, \widehat{\mu}_k$ the complex conjugate ones. Moreover, let

$$\widehat{r}_j = ((\varepsilon + \widehat{a}_j)^2 + \widehat{b}_j^2)^{1/2}, \quad \widehat{R} = \max_{1 \leq j \leq k} \widehat{r}_j,$$

and

$$\widehat{\omega}_k(\varepsilon) = \prod_{j=1}^k (\widehat{r}_j(\varepsilon + \widehat{a}_j))^{1/2}.$$

Define

$$\widehat{\varsigma}_k(\rho) = \prod_{j=1}^{k_2} (1 + \rho^2 / \widehat{r}_j^2)^{1/2} \prod_{j=k_2+1}^k (1 + \rho^2 / \widehat{r}_j^2)^{1/4},$$

and

$$\widehat{d}_k(\rho) = \frac{\prod_{j=1}^{k-1} h_{j+1,j}}{\widehat{\omega}_k(\varepsilon) \widehat{\varsigma}_k(\rho)}.$$

Under these assumptions, we have the following result for the harmonic Arnoldi approximation, whose proof is similar to that of Theorem 4.2.

Theorem 4.5. *Let $\varepsilon > 0$, and suppose that $k + k_2 + 2\ell \geq 4$ and $W(T_k) \subset \Sigma_{\vartheta,a}$. Then for the harmonic Arnoldi approximation, we have*

$$\|\widehat{\mathbf{e}}_{\ell,k}(t)\|_2 \leq \widehat{c}_{\ell,k} \cdot \int_0^\infty \frac{(1 + \rho^2 / \varepsilon^2)^{-\ell/2}}{\widehat{\varsigma}_k(\rho)} d\rho \cdot \|\widehat{\mathbf{r}}_{\ell,k}(t)\|_2 \tag{4.19}$$

where $\widehat{c}_{\ell,k} = \frac{\exp(t\varepsilon)}{\pi(t\varepsilon)^\ell \widehat{\omega}_k(\varepsilon)(\varepsilon+a)} \cdot \frac{\prod_{j=1}^{k-1} h_{j+1,j}}{|\mathbf{e}_k^H \varphi_\ell(-tT_k) \mathbf{e}_1|}$.

The following result avoids the use of a quadrature rule for evaluating the integral in (4.19). The proof is analogous to that of Theorem 4.3.

Theorem 4.6. *Let $\varepsilon > 0$ and suppose that $k + k_2 \geq 4$. Under the above notations, we have that*

$$\|\widehat{\mathbf{e}}_{\ell,k}(t)\|_2 \leq \widehat{c}_{\ell,k} \cdot \widehat{C}_k \cdot \|\widehat{\mathbf{r}}_{\ell,k}(t)\|_2,$$

where

$$\widehat{C}_k = \frac{\sqrt{\pi}}{2\sqrt{\widehat{S}_1}} + \exp(-\varepsilon^2 \widehat{S}_2)(\widehat{R} - \varepsilon) + \left(\frac{\varepsilon}{\sqrt{\varepsilon^2 + \widehat{R}^2}}\right)^\ell \frac{\pi \widehat{R}}{2^{(\frac{k+k_2}{4}+1)}},$$

with

$$\widehat{S}_1 = \frac{\ell}{4\varepsilon^2} + \frac{1}{2} \sum_{j=1}^{k_2} \frac{1}{\widehat{r}_j^2 + \varepsilon^2} + \frac{1}{4} \sum_{j=k_2+1}^k \frac{1}{\widehat{r}_j^2 + \varepsilon^2},$$

and

$$\widehat{S}_2 = \frac{\ell}{2(\varepsilon^2 + \widehat{R}^2)} + \frac{1}{2} \sum_{j=1}^{k_2} \frac{1}{\widehat{r}_j^2 + \widehat{R}^2} + \frac{1}{4} \sum_{j=k_2+1}^k \frac{1}{\widehat{r}_j^2 + \widehat{R}^2}.$$

5 The advantage of the thick-restarting strategy for matrix functions

In this section, we show the advantage of augmenting approximate eigenvectors in the thick-restarted Arnoldi and the harmonic Arnoldi algorithms. For simplicity, we consider the case of augmenting only one (approximate) eigenvector. Let's first discuss an "ideal" case in which an "exact" eigenvector \mathbf{x} is added into the search space. The orthonormal basis is $V_k = [\mathbf{x}, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_k] = [\mathbf{x}, V_\perp]$ after restarting, where $V_\perp = [\mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_k]$ and $A\mathbf{x} = \lambda\mathbf{x}$. Then we have

$$H_k = V_k^H A V_k = \begin{bmatrix} \mathbf{x}^H \\ V_\perp^H \end{bmatrix} \begin{bmatrix} A\mathbf{x} & A V_\perp \end{bmatrix} = \begin{bmatrix} \lambda & \mathbf{x}^H A V_\perp \\ \mathbf{0} & V_\perp^H A V_\perp \end{bmatrix} \equiv \begin{bmatrix} \lambda & H_{12} \\ \mathbf{0} & H_{22} \end{bmatrix}, \quad (5.1)$$

and

$$(zI + tH_k)^{-1} = \begin{bmatrix} (z + t\lambda)^{-1} & \mathbf{s}^H \\ \mathbf{0} & (zI + tV_\perp^H A V_\perp)^{-1} \end{bmatrix},$$

where $\mathbf{s} \in \mathbb{C}^{k-1}$ is a vector. As a result,

$$\mathbf{e}_k^H (zI + tH_k)^{-1} \beta \mathbf{e}_1 = 0,$$

so we have from (4.4) that

$$\mathbf{e}_{\ell,k}(t) = \mathbf{y}(t) - \mathbf{y}_{\ell,k}(t) = \frac{1}{2\pi i} \int_{\Gamma} \varphi_\ell(z) (zI + tA)^{-1} \left[-th_{k+1,k} [\mathbf{e}_k^H (zI + tH_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1} \right] dz = \mathbf{0}. \quad (5.2)$$

Now let's consider the harmonic Arnoldi approximation. If $V_k = [\mathbf{x}, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_k]$, we notice from (5.1) and (3.4) that

$$\mathbf{e}_k^H (zI + tT_k)^{-1} \beta \mathbf{e}_1 = \mathbf{e}_k^H (zI + tH_k)^{-1} \beta \mathbf{e}_1 = 0. \quad (5.3)$$

Consequently, we have from (4.17) that

$$\begin{aligned}
\widehat{\mathbf{e}}_{\ell,k}(t) &= \mathbf{y}(t) - \widehat{\mathbf{y}}_{\ell,k}(t) \\
&= \frac{1}{2\pi i} \int_{\widehat{\Gamma}} \varphi_{\ell}(z)(zI + tA)^{-1} \left[t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1] V_k (I + \gamma H_k)^{-1} \mathbf{e}_k \right. \\
&\quad \left. - th_{k+1,k} [\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1} \right] dz \\
&= \mathbf{0}.
\end{aligned} \tag{5.4}$$

Remark 5.1. Equations (5.2) and (5.4) indicate that, if the search subspace is augmented with an exact eigenvector in the thick-restarted Arnoldi and harmonic Arnoldi algorithms, then we will get the exact solution.

In practical calculations, we are interested in the situation where an approximate eigenvector (say, the Ritz vector or the harmonic Ritz vector) $\tilde{\mathbf{x}}$ is added into the search space spanned by

$$V_k = [\tilde{\mathbf{x}}, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_k] \equiv [\tilde{\mathbf{x}}, V_{\perp}].$$

Let the residual of the Ritz pair $(\tilde{\lambda}, \tilde{\mathbf{x}})$ be $\tilde{\mathbf{r}} = A\tilde{\mathbf{x}} - \tilde{\lambda}\tilde{\mathbf{x}}$, we have

$$H_k = V_k^H A V_k = \begin{bmatrix} \tilde{\mathbf{x}}^H \\ V_{\perp}^H \end{bmatrix} \begin{bmatrix} A\tilde{\mathbf{x}} & AV_{\perp} \end{bmatrix} = \begin{bmatrix} \mu & \tilde{\mathbf{x}}^H AV_{\perp} \\ V_{\perp}^H \tilde{\mathbf{r}} & V_{\perp}^H AV_{\perp} \end{bmatrix} \equiv \begin{bmatrix} \mu & \tilde{H}_{12} \\ V_{\perp}^H \tilde{\mathbf{r}} & H_{22} \end{bmatrix},$$

where we used $V_{\perp}^H A\tilde{\mathbf{x}} = V_{\perp}^H (\tilde{\mathbf{r}} + \tilde{\lambda}\tilde{\mathbf{x}}) = V_{\perp}^H \tilde{\mathbf{r}}$, and $\mu = \tilde{\mathbf{x}}^H A\tilde{\mathbf{x}}$ is a scalar. As only one approximate eigenvector is added into V_k , we see that H_k is still an upper Hessenberg matrix. Denote by $h_{2,1}$ the $(2, 1)$ element of H_k , then $V_{\perp}^H \tilde{\mathbf{r}} = [h_{2,1}, 0, \dots, 0]^H$ and

$$|h_{2,1}| = \|V_{\perp}^H \tilde{\mathbf{r}}\|_2 \leq \|\tilde{\mathbf{r}}\|_2. \tag{5.5}$$

Let

$$\tilde{Q} = (zI + tH_k) - th_{2,1} \mathbf{e}_2 \mathbf{e}_1^H, \tag{5.6}$$

note that \tilde{Q} is an upper Hessenberg matrix with its $(2, 1)$ element being zero. If \tilde{Q} is nonsingular and $th_{2,1}(\mathbf{e}_1^H \tilde{Q}^{-1} \mathbf{e}_2) \neq -1$, by the Sherman–Morrison formula [23], we obtain

$$\begin{aligned}
\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1 &= \mathbf{e}_k^H(\tilde{Q} + th_{2,1} \mathbf{e}_2 \mathbf{e}_1^H)^{-1} \beta \mathbf{e}_1 \\
&= -\frac{th_{2,1} \beta(z + t\mu)^{-1}}{1 + th_{2,1}(\mathbf{e}_1^H \tilde{Q}^{-1} \mathbf{e}_2)} \cdot (\mathbf{e}_k^H \tilde{Q}^{-1} \mathbf{e}_2) \\
&\equiv h_{2,1} \cdot \xi(z),
\end{aligned} \tag{5.7}$$

where

$$\xi(z) = -\frac{t\beta(z + t\mu)^{-1}}{1 + th_{2,1}(\mathbf{e}_1^H \tilde{Q}^{-1} \mathbf{e}_2)} \cdot (\mathbf{e}_k^H \tilde{Q}^{-1} \mathbf{e}_2). \tag{5.8}$$

So we have

$$\begin{aligned}
\|\mathbf{e}_{\ell,k}(t)\|_2 &= \left\| \frac{1}{2\pi i} \int_{\Gamma} \varphi_{\ell}(z)(zI + tA)^{-1} \left[-th_{k+1,k} [\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1} \right] dz \right\|_2 \\
&= |th_{k+1,k} h_{2,1}| \cdot \left\| \frac{1}{2\pi i} \int_{\Gamma} \varphi_{\ell}(z)(zI + tA)^{-1} \cdot \xi(z) \mathbf{v}_{k+1} dz \right\|_2.
\end{aligned} \tag{5.9}$$

By (5.9) and (5.5), we have the following theorem. It shows the advantage of augmenting a Ritz vector in the search space of the thick-restarted Arnoldi method.

Theorem 5.1. *Let $(\tilde{\lambda}, \tilde{\mathbf{x}})$ be a Ritz pair with residual $\tilde{\mathbf{r}}$, and let $V_k = [\tilde{\mathbf{x}}, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_k]$. Then in the thick-restarted Arnoldi algorithm, we have*

$$\|\mathbf{e}_{\ell,k}(t)\|_2 \leq \|\tilde{\mathbf{r}}\|_2 \cdot |th_{k+1,k}| \left\| \frac{1}{2\pi i} \int_{\Gamma} \varphi_{\ell}(z)(zI + tA)^{-1} \cdot \xi(z) \mathbf{v}_{k+1} dz \right\|_2. \quad (5.10)$$

Next we consider the thick-restarted harmonic Arnoldi algorithm. For simplicity, we still denote $V_k = [\tilde{\mathbf{x}}, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_k]$, whose columns span the search subspace; and let the residual of the harmonic Ritz pair $(\tilde{\lambda}, \tilde{\mathbf{x}})$ be $\tilde{\mathbf{r}} = A\tilde{\mathbf{x}} - \tilde{\lambda}\tilde{\mathbf{x}}$. If $1 + t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H(zI + tH_k)^{-1}(I + \gamma H_k)^{-H} \mathbf{e}_k] \neq 0$, we obtain from (3.4) and the Sherman–Morrison formula that

$$\begin{aligned} \mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1 &= \mathbf{e}_k^H \left[(zI + tH_k)^{-1} \beta \mathbf{e}_1 - [1 + t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H(zI + tH_k)^{-1}(I + \gamma H_k)^{-H} \mathbf{e}_k]]^{-1} \right. \\ &\quad \left. (zI + tH_k)^{-1} t\gamma h_{k+1,k}^2 (I + \gamma H_k)^{-H} \mathbf{e}_k [\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1] \right] \\ &= [1 - \zeta_1(z)\zeta_2(z)] [\mathbf{e}_k^H(zI + tH_k)^{-1} \beta \mathbf{e}_1], \end{aligned} \quad (5.11)$$

where

$$\zeta_1(z) = [1 + t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H(zI + tH_k)^{-1}(I + \gamma H_k)^{-H} \mathbf{e}_k]]^{-1},$$

and

$$\zeta_2(z) = t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H(zI + tH_k)^{-1}(I + \gamma H_k)^{-H} \mathbf{e}_k].$$

Therefore, we have from (5.7) and (5.11) that

$$\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1 = [1 - \zeta_1(z)\zeta_2(z)] \xi(z) h_{2,1} \equiv \chi(z) h_{2,1}, \quad (5.12)$$

and

$$|\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1| \leq |\chi(z)| \cdot \|\tilde{\mathbf{r}}\|_2.$$

Denote

$$\mathbf{c}_{k+1}(z) = \begin{bmatrix} \gamma h_{k+1,k} \chi(z) (I + \gamma H_k)^{-H} \mathbf{e}_k \\ -\chi(z) \end{bmatrix},$$

from the relations (4.17) and (5.12), we get

$$\begin{aligned} \|\widehat{\mathbf{e}}_{\ell,k}(t)\|_2 &= \left\| \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_{\ell}(z)(zI + tA)^{-1} \left[t\gamma h_{k+1,k}^2 [\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1] V_k (I + \gamma H_k)^{-1} \mathbf{e}_k \right. \right. \\ &\quad \left. \left. - th_{k+1,k} [\mathbf{e}_k^H(zI + tT_k)^{-1} \beta \mathbf{e}_1] \mathbf{v}_{k+1} \right] dz \right\|_2 \\ &= \left\| \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_{\ell}(z)(zI + tA)^{-1} \left[t\gamma h_{k+1,k}^2 [\chi(z) h_{2,1}] V_k (I + \gamma H_k)^{-H} \mathbf{e}_k \right. \right. \\ &\quad \left. \left. - th_{k+1,k} [\chi(z) h_{2,1}] \mathbf{v}_{k+1} \right] dz \right\|_2 \\ &= \left\| th_{k+1,k} h_{2,1} \cdot \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_{\ell}(z)(zI + tA)^{-1} \cdot V_{k+1} \mathbf{c}_{k+1}(z) dz \right\|_2. \end{aligned} \quad (5.13)$$

From (5.13) and (5.5), we obtain the following theorem. It shows the merit of augmenting a harmonic Ritz vector in the search space of the thick-restarted harmonic Arnoldi method.

Theorem 5.2. *Let $(\tilde{\lambda}, \tilde{\mathbf{x}})$ be a harmonic Ritz pair with residual $\tilde{\mathbf{r}}$, and let $V_k = [\tilde{\mathbf{x}}, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_k]$. Then in the thick-restarted harmonic Arnoldi algorithm, we have*

$$\|\widehat{\mathbf{e}}_{\ell,k}(t)\|_2 \leq \|\tilde{\mathbf{r}}\|_2 \cdot |th_{k+1,k}| \left\| \frac{1}{2\pi i} \int_{\hat{\Gamma}} \varphi_{\ell}(z)(zI + tA)^{-1} \cdot V_{k+1} \mathbf{c}_{k+1}(z) dz \right\|_2. \quad (5.14)$$

6 Numerical experiments

In this section, we make some numerical experiments to show the superiority of our new algorithm over many state-of-the-art algorithms for computing φ -functions. The numerical experiments are run on a Dell PC with eight core Intel(R) Core(TM)i7-2600 processor with CPU 3.40 GHz and RAM 16.0 GB, under the Windows 7 with 64-bit operating system. All the numerical results are obtained from using a MATLAB 7.10.0 implementation with machine precision $\epsilon \approx 2.22 \times 10^{-16}$. The algorithms used in this section are listed as follows.

- **phipm** [48] computes the action of linear combinations of φ -functions on operand vectors. The implementation combines time stepping with a procedure to adapt the Krylov subspace size. The MATLAB codes are available from <http://www1.maths.leeds.ac.uk/~jitse/software.html>.

- **expv** is the MATLAB function due to Sidje [57], which evaluates $\exp(-tA)\mathbf{v}$ using a restarted Krylov subspace method with a fixed dimension. The MATLAB codes are available from <http://www.maths.uq.edu.au/expokit/>.

- **funm_kryl** is a realization of the Krylov subspace method with deflated restarting for matrix functions [15]. Its effect is to ultimately deflate a specific invariant subspace of the matrix which most impedes the convergence of the restarted Arnoldi approximation process. The MATLAB codes are available from http://www.mathe.tu-freiberg.de/~guettels/funm_kryl/.

- **funm_quad** is a realization of the restarted Arnoldi algorithm described in [18]. This algorithm utilizes an integral representation for the error of the iterates in the Arnoldi method which then allows one to develop a quadrature-based restarting algorithm suitable for a large class of functions. It can be viewed as an improved version of the deflated restarting Krylov algorithm proposed in [15]. The MATLAB codes can be downloaded from http://www.guettel.com/funm_quad.

- **Rich_Kryl** is the restarted and residual-based Krylov-Richardson algorithm for computing the matrix exponential problem $\exp(-tA)\mathbf{v}$ [8].

- **TRA** and **TRHA** are the thick-restarted Arnoldi algorithm and the thick-restarted harmonic Arnoldi algorithm (Algorithm 1), respectively, for evaluating $\varphi_\ell(-tA)\mathbf{v}$, $\ell = 0, 1, \dots, s$.

We run the MATLAB functions *phipm*, *expv*, *funm_kryl* and *funm_quad* using their default parameters. In all the algorithms, the convergence tolerance for φ -functions is chosen as $tol = 10^{-8}$, and the dimension k for the Krylov subspace is set to be 30. In the deflated Krylov subspace algorithms *funm_kryl*, *funm_quad*, TRA and TRHA, we set the number q of approximate eigenvectors retained from the previous cycles to be 5, and augment the search subspace with approximate eigenvectors corresponding to the smallest approximate eigenvalues. The parameter γ in TRHA is set to be $\gamma = 0.01t$ in all the numerical examples. For the reduced matrices (projection matrices), the matrix exponential are computed by using the MATLAB built-in function *expm*, and the φ_ℓ ($\ell \geq 1$) functions are computed by using the *phipade* function of the EXPINT package available from <http://www.math.ntnu.no/num/expint/>.

In the residual-based algorithms Rich_Kryl, TRA and TRHA, we solve the initial value problems by using the *ode15s* ODE solver in MATLAB, whose absolute and relative tolerances are chosen as 10^{-9} . In the tables below, we denote by “CPU” the CPU time in seconds, and by “Mv” the number of matrix-vector products. Let $\mathbf{y}(t)$ be the “exact” solution, and let $\tilde{\mathbf{y}}(t)$ be an approximation obtained from running the above algorithms, then we define the relative error

$$\mathbf{Error} = \frac{\|\mathbf{y}(t) - \tilde{\mathbf{y}}(t)\|_2}{\|\mathbf{y}(t)\|_2}.$$

If an algorithm does not converge within an acceptable CPU timing (say, 6 hours), then we stop and declare that the algorithm “fails to converge”.

Example 6.1. In this example, we compare TRHA with *phipm*, *funm_kryl* and TRA for the computation of φ -functions, and show the efficiency of our new algorithm for solving (1.3) *simultaneously*. The test problem is routinely used to study performance of stiff integrators [26, 61]. Consider the following two-dimensional semilinear reaction-diffusion-advection equation

$$u_t = \varepsilon_1(u_{xx} + u_{yy}) - \beta_1(u_x + u_y) + \rho_1 u(u - \frac{1}{2}(1 - u)) \quad (6.1)$$

defined on the unit square $\Omega = [0, 1]^2$, which satisfies the homogeneous Dirichlet boundary conditions. We set $\varepsilon_1 = 0.02$, $\beta_1 = -0.02$, $\rho_1 = 1$, and use

$$u(t = 0, x, y) = 256(xy(1 - x)(1 - y))^2 + 0.3$$

as the initial condition.

ℓ	Algorithm	CPU	Error	Mv
0	phipm	151.11	4.757×10^{-13}	3389
	funm_kryl	168.03	8.000×10^{-12}	1355
	TRA	178.22	5.277×10^{-9}	1780
	TRHA	163.17	1.413×10^{-8}	1630
1	phipm	163.61	2.069×10^{-13}	2408
	funm_kryl	221.22	7.116×10^{-12}	1255
	TRA	159.58	1.513×10^{-9}	1655
	TRHA	145.71	1.179×10^{-9}	1505
2	phipm	148.03	4.198×10^{-13}	2149
	funm_kryl	249.28	1.347×10^{-11}	1155
	TRA	145.02	3.007×10^{-9}	1530
	TRHA	131.26	1.703×10^{-9}	1380
3	phipm	138.88	9.892×10^{-14}	2035
	funm_kryl	236.98	3.703×10^{-11}	1055
	TRA	133.23	8.363×10^{-9}	1405
	TRHA	119.95	4.685×10^{-9}	1280
total	phipm	601.63	–	9981
	funm_kryl	875.50	–	4820
	TRA	616.04	–	6370
	TRHA	560.08	–	5795

Example 6.1. Table 1: Numerical results of the 2D reaction-diffusion-advection equation (6.1), the matrix size $n = N^2 = 250,000$. Compute $\varphi_\ell(-tA)\mathbf{u}_0$, $\ell = 0, 1, 2, 3$ *sequentially* (one by one) by using TRA, TRHA, *phipm* and *funm_kryl*.

We discretize (6.1) spatially by standard finite differences with meshwidth $\Delta x = \Delta y = \frac{1}{N+1}$ and $N = 500$. This gives a system of ODEs of size N^2 :

$$\mathbf{u}'(t) = -A\mathbf{u}(t) + \mathbf{f}(\mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0.$$

This linear differential system can be efficiently solved by means of the exponential Runge-Kutta integrators [33]. More precisely, $\mathbf{u}(t_{\hat{n}+1})$ can be approximated from $t_{\hat{n}}$ to $t_{\hat{n}+1} = t_{\hat{n}} + \Delta t$ ($\hat{n} = 0, 1, 2, \dots$) by $\mathbf{u}_{\hat{n}+1}$ defined as

$$\mathbf{u}_{\hat{n}+1} = \mathbf{u}_{\hat{n}} + \Delta t \sum_{i=1}^{\hat{s}} c_i (-\Delta t A) (\mathbf{f}_{\hat{n}i} - A \mathbf{u}_{\hat{n}}),$$

where

$$\mathbf{f}_{\hat{n}i} = \mathbf{f}(\mathbf{U}_{\hat{n}i}), \quad i = 1, \dots, \hat{s},$$

with

$$\mathbf{U}_{\hat{n}i} = \mathbf{u}_{\hat{n}} + \Delta t \sum_{j=1}^{i-1} a_{ij} (-\Delta t A) (\mathbf{f}_{\hat{n}j} - A \mathbf{u}_{\hat{n}}),$$

and the coefficients c_i, a_{ij} are constructed from the φ -functions. If Krogstad's four-stage scheme (see [38] and Example 2.19 of [33]) is used to integrate the system of ODEs, one needs to compute the terms $\varphi_{\ell}(-\Delta t A)(\mathbf{f}_{\hat{n}1} - A \mathbf{u}_{\hat{n}})$ with $\ell = 1, 2, 3$ simultaneously in each time step. Similarly, if the generalized Lawson scheme (see Example 2.34 of [33]) is used, the vectors $\varphi_{\ell}(-\frac{\Delta t}{2} A) \hat{\mathbf{v}}$ with $\ell = 0, 1, 2$ are necessary to be approximated for the same vector $\hat{\mathbf{v}}$ in each time step.

In this example, we want to compute $\varphi_{\ell}(-tA)\mathbf{u}_0$ with $\ell = 0, 1, 2, 3$ and $t = 1$. Here the "exact" solutions are obtained from running the MATLAB function *phipm* with convergence tolerance $tol = 10^{-14}$. In Table 1, we list the CPU time and the number of matrix-vector products for computing the four vectors *sequentially* (one by one); while in Table 2, we present those for evaluating the four vectors *simultaneously*. So as to illustrate the merit of TRHA for solving the four vectors simultaneously, in Table 1, we also list the total CPU time and the total number of matrix-vector products for computing the four vectors sequentially.

ℓ	Algorithm	CPU	Error	Mv
0 ~ 3	funm_kryl	663.25	8.000×10^{-12}	1355
			2.454×10^{-13}	
			1.171×10^{-13}	
			8.952×10^{-14}	
0 ~ 3	TRA	204.91	5.277×10^{-9}	1780
			1.513×10^{-9}	
			3.007×10^{-9}	
			8.363×10^{-9}	
0 ~ 3	TRHA	191.14	1.413×10^{-8}	1630
			1.180×10^{-9}	
			1.703×10^{-9}	
			4.685×10^{-9}	

Example 6.1. Table 2: Numerical results of the 2D reaction-diffusion-advection equation (6.1), the matrix size $n = N^2 = 250,000$. Compute $\varphi_{\ell}(-tA)\mathbf{u}_0$, $\ell = 0, 1, 2, 3$ *simultaneously* by using TRA, TRHA and *funm_kryl*.

Three remarks are in order. First, we observe from Table 1 and Table 2 that, whether this problem is solved sequentially or simultaneously, TRHA always works better than the other algorithms in terms of CPU time, especially when ℓ is large. Second, it is seen that when this problem is solved simultaneously, the total CPU time of TRHA are much less than those of *phipm* and *funm_kryl*. More precisely, we can save about $\frac{2}{3}$ CPU time, 191.14 seconds vs. 601.63 and 663.25 seconds. However, we find that the number of matrix-vector products of *phipm* is less than those of TRA and TRHA. Indeed, solving small ODE problems during cycles is a large overhead for TRA and TRHA, and the number of matrix-vector products is not the whole story for accessing the computational complexities. Third, the accuracy of the approximations obtained from *phipm* and *funm_kryl* can be (much) higher than that obtained from TRA and TRHA. The reason is due to the fact that we need to solve a small-sized ODE problem during each cycle of the residual based algorithms.

ℓ	Algorithm	CPU	Error	Mv
1	phipm	171.07	1.356×10^{-14}	2477
	funm_kryl	198.80	1.338×10^{-11}	1205
	TRA	147.50	1.946×10^{-10}	1555
	TRHA	137.20	1.122×10^{-10}	1455
2	phipm	154.43	2.977×10^{-13}	2239
	funm_kryl	185.29	3.529×10^{-11}	1055
	TRA	133.55	3.124×10^{-10}	1430
	TRHA	121.45	1.898×10^{-10}	1305
3	phipm	135.28	2.564×10^{-12}	2448
	funm_kryl	161.12	7.971×10^{-11}	930
	TRA	119.02	1.520×10^{-9}	1280
	TRHA	107.43	9.209×10^{-10}	1155
4	phipm	137.17	4.843×10^{-13}	2844
	funm_kryl	124.83	2.715×10^{-10}	805
	TRA	105.40	6.177×10^{-9}	1130
	TRHA	95.48	4.213×10^{-9}	1030
total	phipm	597.95	–	10008
	funm_kryl	670.04	–	3995
	TRA	505.47	–	5395
	TRHA	461.55	–	4945

Example 6.2. Table 3: Numerical results of the problem (6.2), the matrix size $n = N^2 = 250,000$. Compute $\varphi_\ell(-t\hat{A})\mathbf{v}$, $\ell = 1, 2, 3, 4$ *sequentially* (one by one) by using *phipm*, *funm_kryl*, TRA and TRHA.

Example 6.2. In this example, we consider the following stiff problems [22]

$$\mathbf{y}'(t) = -A\mathbf{y}(t) + \frac{t^{\ell-1}}{(\ell-1)!}\mathbf{v}, \quad \mathbf{y}(0) = \mathbf{0}, \quad \ell = 1, 2, \dots, s. \quad (6.2)$$

The exact solutions at time t are $\mathbf{y}(t) = t^\ell \varphi_\ell(-tA)\mathbf{v}$, $\ell = 1, 2, \dots, s$. Therefore, we need to solve the s vectors simultaneously. In this example, the matrix $-A \in \mathbb{R}^{n \times n}$ is the standard finite difference discretization matrix for the two-dimensional Laplacian on the unit square with homogeneous Dirichlet

boundary conditions, where we use a regular grid with $n = N^2$ inner discretization points and mesh size $h = \frac{1}{N+1}$. The vector $\mathbf{v} = (g(ih, jh))_{i,j=1}^N$ contains the evaluations of the function $g(x, y) = 30x(1 - x)y(1 - y)$ at the inner grid points. We compute $\mathbf{y}(t) = \varphi_\ell(-t\hat{A})\mathbf{v}$, $\ell = 1, 2, 3, 4$ with $\hat{A} = 0.025 \times A$ and $t = 1$. The “exact” solutions are obtained from running *hipm* with the convergence tolerance $tol = 10^{-14}$.

It is seen from Tables 3–4 that both TRA and TRHA outperform the other algorithms, and we benefit from the thick-restarting strategy. Specifically, when the vectors are computed simultaneously, TRHA works much better than *funm_kryl* and *hipm* in terms of CPU time, 154.09 seconds vs. 462.72 and 597.95 seconds, a great improvement. On the other hand, we observe from the two tables that TRHA performs better than TRA in terms of both CPU time and the number of matrix-vector products. Furthermore, the accuracy of the approximations got from TRHA is a little higher than that of TRA. All these show the superiority of the harmonic projection technique over the orthogonal projection technique for φ -functions.

ℓ	Algorithm	CPU	Error	Mv
1 ~ 4	funm_kryl	462.72	1.338×10^{-11} 1.204×10^{-12} 2.249×10^{-13} 1.395×10^{-13}	1205
1 ~ 4	TRA	164.71	1.946×10^{-10} 3.126×10^{-10} 1.520×10^{-9} 6.177×10^{-9}	1555
1 ~ 4	TRHA	154.09	1.122×10^{-10} 1.908×10^{-10} 9.217×10^{-10} 4.213×10^{-9}	1455

Example 6.2. Table 4: Numerical results of the problem (6.2), the matrix size $n = N^2 = 250,000$. Compute $\varphi_\ell(-t\hat{A})\mathbf{v}$, $\ell = 1, 2, 3, 4$ *simultaneously* by using *funm_kryl*, TRA and TRHA.

Example 6.3. This test problem is the *G2_circuit* matrix arising from the circuit simulation problem. It is size of $150,102 \times 150,102$, with 726,674 nonzero elements, whose data file is available from the University of Florida Sparse Matrix Collection: <http://www.cise.ufl.edu/research/sparse/matrices>. In this example, we want to compute $\varphi_\ell(-A)\mathbf{v}$, $\ell = 0, 1, 2, 3$ with $A = 10 \times G2_circuit$ and $\mathbf{v} = [1, 1, \dots, 1]^T$, by using *hipm*, *funm_kryl*, TRA and TRHA. The “exact” solutions are got from running *hipm* with the convergence tolerance $tol = 10^{-14}$. Tables 5 and 6 list the numerical results.

Again, it is observed from Tables 5–6 that TRHA works much better than the other algorithms in terms of CPU time, especially when the vectors are computed simultaneously. However, the accuracy of the approximations obtained from *hipm* and *funm_kryl* can be (much) higher than that obtained from TRA and TRHA. As we have mentioned before, the reason is due to the fact that one needs to solve a small-sized ODE problem inexactly during each cycle of the two residual-based algorithms. Therefore, if accuracy is not the most important thing and one wants to solve (1.3) rapidly, TRHA is a competitive candidate for the φ -functions of very large matrices.

ℓ	Algorithm	CPU	Error	Mv
0	phipm	121.43	8.843×10^{-14}	4982
	funm_kryl	445.84	1.573×10^{-11}	1880
	TRA	153.04	6.406×10^{-9}	2780
	TRHA	125.48	8.892×10^{-9}	2380
1	phipm	130.30	2.890×10^{-14}	3144
	funm_kryl	689.39	7.898×10^{-12}	1755
	TRA	137.60	2.401×10^{-9}	2630
	TRHA	110.82	1.668×10^{-9}	2230
2	phipm	115.80	6.714×10^{-13}	2820
	funm_kryl	763.95	1.967×10^{-11}	1605
	TRA	126.84	4.788×10^{-9}	2480
	TRHA	100.34	2.982×10^{-9}	2080
3	phipm	107.20	6.643×10^{-12}	2621
	funm_kryl	698.22	1.020×10^{-10}	1430
	TRA	115.23	1.259×10^{-8}	2280
	TRHA	90.58	8.306×10^{-9}	1905
total	phipm	474.74	–	13567
	funm_kryl	2597.40	–	6670
	TRA	532.71	–	10170
	TRHA	427.21	–	8595

Example 6.3. Table 5: Numerical results of computing $\varphi_\ell(-A)\mathbf{v}$, $\ell = 0, 1, 2, 3$ *sequentially* (one by one) by using *phipm*, *funm_kryl*, TRA and TRHA. The matrix $A = 10 \times G2_circuit$, which is of size $n = 150, 102$.

p	Algorithm	CPU	Error	Mv
0 ~ 3	funm_kryl	2220.20	1.573×10^{-11}	1880
			6.834×10^{-13}	
			4.309×10^{-13}	
			3.169×10^{-13}	
0 ~ 3	TRA	187.27	6.406×10^{-9}	2780
			2.401×10^{-9}	
			4.788×10^{-9}	
			1.259×10^{-8}	
0 ~ 3	TRHA	157.04	8.892×10^{-9}	2380
			1.667×10^{-9}	
			2.982×10^{-9}	
			8.306×10^{-9}	

Example 6.3. Table 6: Numerical results of computing $\varphi_\ell(-A)\mathbf{v}$, $\ell = 0, 1, 2, 3$ *simultaneously* by using *funm_kryl*, TRA and TRHA. The matrix $A = 10 \times G2_circuit$, which is of size $n = 150, 102$.

Example 6.4. In this example, the test matrix is generated by using the MATLAB function “gallery”: $A = -\text{gallery}('lesp', 6000)$. It returns a 6000×6000 tridiagonal matrix with real, sensitive eigenvalues. We compute $\varphi_\ell(-A)\mathbf{v}$, $\ell = 1, 2, 3, 4$ by *phipm*, *funm_kryl*, TRA and TRHA, where \mathbf{v} is set to be the vector of all ones. The “exact” solutions are derived from running the MATLAB function *phipade* of the EXPINT package [6]. Tables 7–8 list the numerical results.

It is seen from the numerical results that TRHA still works quite well for the matrix with sensitive eigenvalues. Indeed, TRA and TRHA outperform *phipm* and *funm_kryl* considerably in terms of CPU time, while TRHA performs the best in many cases. Furthermore, one can save about one half of CPU time if the 4 vectors are computed simultaneously instead of sequentially. For this test problem, if the vectors are evaluated one by one, we observe from Table 7 that the accuracy of the approximations obtained from TRA and TRHA is comparable to that of the approximations from running *funm_kryl*.

ℓ	Algorithm	CPU	Error	Mv
1	phipm	50.03	2.824×10^{-10}	2572
	funm_kryl	110.79	6.538×10^{-9}	1055
	TRA	31.88	2.546×10^{-8}	1280
	TRHA	30.54	1.508×10^{-8}	1205
2	phipm	44.67	1.986×10^{-10}	2273
	funm_kryl	108.58	1.096×10^{-8}	930
	TRA	27.16	3.085×10^{-8}	1180
	TRHA	25.97	2.343×10^{-8}	1105
3	phipm	42.36	1.209×10^{-9}	2131
	funm_kryl	96.94	1.864×10^{-8}	830
	TRA	24.45	1.210×10^{-7}	1080
	TRHA	22.93	7.545×10^{-8}	1005
4	phipm	42.78	8.563×10^{-10}	2145
	funm_kryl	77.03	4.985×10^{-8}	730
	TRA	21.57	5.240×10^{-7}	955
	TRHA	19.89	3.367×10^{-7}	880
total	phipm	179.84	–	9121
	funm_kryl	393.34	–	3545
	TRA	105.05	–	4495
	TRHA	99.33	–	4195

Example 6.4. Table 7: Numerical results of computing $\varphi_\ell(-A)\mathbf{v}$, $\ell = 1, 2, 3, 4$ *sequentially* (one by one) by using *phipm*, *funm_kryl*, TRA and TRHA. The matrix $A = -\text{gallery}('lesp', 6000)$, which is of size $n = 6000$.

ℓ	Algorithm	CPU	Error	Mv
1 ~ 4	funm_kryl	267.98	6.538×10^{-9} 4.259×10^{-10} 4.617×10^{-11} 6.551×10^{-12}	1055
1 ~ 4	TRA	42.29	2.546×10^{-8} 3.088×10^{-8} 1.209×10^{-7} 5.240×10^{-7}	1280
1 ~ 4	TRHA	40.49	1.508×10^{-8} 2.364×10^{-8} 7.524×10^{-8} 3.364×10^{-7}	1205

Example 6.4. Table 8: Numerical results of computing $\varphi_\ell(-A)\mathbf{v}$, $\ell = 1, 2, 3, 4$ *simultaneously* by using *funm_kryl*, TRA and TRHA. The matrix $A = -\text{gallery}('lesp', 6000)$, which is of size $n = 6000$.

Since the computation of φ -functions can be rewritten in terms of a single matrix exponential by considering a slightly augmented matrix [2, 54, 57], it is interesting to investigate the numerical approximation of the matrix exponential applied to a vector. In the following two examples, we try to compare our TRHA algorithm with some state-of-the-art algorithms, such as *expv*, *hipm*, *funm_kryl* and *funm_quad* for matrix exponential.

Example 6.5. In this example, we compare our TRHA algorithm with *expv*, *funm_kryl*, *funm_quad*, *Rich_Kry* and TRA, and show the efficiency of the new algorithm for matrix exponential. In this example, the “exact” solutions are derived from running the MATLAB built-in function *expm.m*.

There are two test problems in this example. The first one is from [39]. We consider pricing options for a single underlying asset in Merton’s jump-diffusion model [41]. In Merton’s model, jumps are normally distributed with mean $\hat{\mu}$ and variation σ . The option value $w(\xi, \tau)$ with logarithmic price ξ and backward time τ satisfies a forward PIDE on $(-\infty, +\infty) \times [0, t]$:

$$w_\tau = \frac{\nu^2}{2} w_{\xi\xi} + (r - \hat{\lambda}\kappa - \frac{\nu^2}{2}) w_\xi - (r + \hat{\lambda})w + \hat{\lambda} \int_{-\infty}^{\infty} w(\xi + \eta, \tau) \phi(\eta) d\eta, \quad (6.3)$$

where t is the maturity time, ν is the stock return volatility, r is the risk-free interest rate, $\hat{\lambda}$ is the arrival intensity of a Poisson process, $\kappa = \exp(\hat{\mu} + \frac{\sigma^2}{2}) - 1$ is the expectation of the impulse function, and ϕ is the Gaussian distribution given by

$$\phi(\eta) = \frac{\exp(-(\eta - \hat{\mu})^2/2\sigma^2)}{\sqrt{2\pi}\sigma}.$$

For a European call option, the initial condition is

$$w(\xi, 0) = \max(K \exp(\xi) - K, 0), \quad (6.4)$$

where K is the strike price [41]. Similar to [39], we truncate the ξ -domain $(-\infty, \infty)$ to $[\xi_1, \xi_2]$ and then divide $[\xi_1, \xi_2]$ into $n + 1$ subintervals with a uniform mesh size h_ξ . By approximating the differential part

of (6.3) by central difference discretization, we can obtain an $n \times n$ tridiagonal Toeplitz matrix \mathcal{D}_n . For the integral term in (6.3), the localized part can be expressed in discrete form by using the rectangle rule. The corresponding operator is an $n \times n$ Toeplitz matrix \mathcal{I}_n . Then the real nonsymmetric Toeplitz matrix $A = -\mathcal{D}_n - \hat{\lambda}\mathcal{I}_n$ is the coefficient matrix of the semidiscretized system with regard to τ . The option price at $\tau = t$ requires evaluating the exponential term $\exp(-tA)\mathbf{w}$, where \mathbf{w} is the discretized form of the initial value in (6.4); see [39] for more details. The input parameters of this problem are $\xi_1 = -2$, $\xi_2 = 2$, $K = 100$, $\nu = 0.25$, $r = 0.05$, $\hat{\lambda} = 0.1$, $\hat{\mu} = -0.9$ and $\sigma = 0.45$. Table 9 presents the numerical results of this problem when $t = 1$ and $n = 4000$.

Algorithm	CPU	Error	Mv
expv	188.09	1.173×10^{-11}	23188
funm_kryl	3894.90	1.191×10^{-11}	3505
funm_quad	n.c.	n.c.	n.c.
Rich_Kryl	202.56	1.990×10^{-8}	5700
TRA	118.27	9.003×10^{-9}	5430
TRHA	115.83	1.836×10^{-9}	4805

Example 6.5. Table 9: Numerical results of the six algorithms on the first test problem, where “n.c.” denotes “fails to converge”.

The second test problem is from numerical solution of the following fractional diffusion equation [51, 63]:

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} - d_+(x) \frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} - d_-(x) \frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} = f(x,t), \\ x \in (0, 2), \quad t \in (0, 1], \\ u(0, t) = u(2, t) = 0, \quad t \in [0, 1], \\ u(x, 0) = u_0(x), \quad x \in [0, 2]. \end{cases} \quad (6.5)$$

In this equation, we set the the coefficients

$$d_+(x) = \frac{\text{Gamma}(3 - \alpha)}{100} x^\alpha,$$

and

$$d_-(x) = \frac{\text{Gamma}(3 - \alpha)}{100} (2 - x)^\alpha,$$

where $1 < \alpha < 2$ and *Gamma* is the Gamma function. We refer to [52] for the definition of the fractional order derivative. After spatial discretization by using the shifted Grünwald formula [40], the equation (6.5) reduces to a semidiscretized ordinary differential equation with the coefficient matrix $A_h = -\frac{1}{h^\alpha}(D_+G + D_-G^T)$, where h is the spatial grid size, D_+ and D_- are diagonal matrices arising from the discretization of the diffusion coefficient $d_+(x)$ and $d_-(x)$, and G is a lower Hessenberg Toeplitz matrix generated by the discretization of the fractional derivative. In this experiment, we choose $\alpha = 1.8$, $t = 1$, and compute $\exp(-tA_h)\mathbf{v}$ with \mathbf{v} being the vector of all ones and the size of the matrix being $n = 4000$. Table 10 lists the numerical results.

Algorithm	CPU	Error	Mv
expv	130.21	4.717×10^{-11}	15872
funm_kryl	2154.30	1.230×10^{-10}	3030
funm_quad	63.72	4.320×10^{-11}	3230
Rich_Kryl	109.28	1.066×10^{-7}	5280
TRA	73.37	3.009×10^{-8}	4555
TRHA	69.96	1.941×10^{-8}	4080

Example 6.5. Table 10: Numerical results of the six algorithms on the second test problem.

Two remarks are given. First, we see from Tables 9 and 10 that TRHA outperforms the other algorithms in terms of CPU time in most cases. In particular, we observe that TRA and TRHA perform much better than *Rich_Kryl* in terms of CPU time and the number of matrix-vector products. This shows that the convergence speed of the Krylov subspace algorithm can be improved significantly by using the thick-restarting strategy. Second, similar to the above numerical experiments, we notice that the accuracy of the approximations obtained from *expv*, *funm_quad* and *funm_kryl* can be (much) higher than that from the residual based algorithms *Rich_Kryl*, TRA and TRHA. As we have mentioned before, the reason is due to the fact that we have to solve a small-sized ODE problem with the tolerance being 10^{-9} in each cycle of the residual-based algorithms.

Example 6.6. In this example, we consider the matrix exponential problem of a large matrix. The test matrix A is the *apache1* matrix arising from the structural problem. It is of size 80800×80800 , with 542184 nonzero elements. The data file is available from the University of Florida Sparse Matrix Collection: <http://www.cise.ufl.edu/research/sparse/matrices>. In this example, we try to evaluate $\exp(-A)\mathbf{v}$ with \mathbf{v} being the vector of all ones. Table 11 reports the numerical results.

Algorithm	CPU	Error	Mv
expv	74.44	8.424×10^{-12}	11036
funm_kryl	695.72	6.719×10^{-11}	2155
funm_quad	n.c.	n.c.	n.c.
Rich_Kry	83.50	5.688×10^{-9}	3600
TRA	85.34	1.627×10^{-9}	3430
TRHA	73.38	1.003×10^{-9}	3005

Example 6.6. Table 11: Numerical results of the six algorithms on $\exp(-A)\mathbf{v}$, where “n.c.” denotes “fails to converge”.

As the MATLAB function *expm.m* is infeasible for very large matrices, in this example, we use the MATLAB function *expmv_tspan* [3] to compute the “exact” solution of the exponential function. The MATLAB codes are available from <http://www.maths.manchester.ac.uk/~almohy/papers.html>. Again, the numerical results show that our new algorithm is superior to the other algorithms in terms of CPU time, and the residual-based TRA and TRHA algorithms are suitable for exponential of very large matrices. Specifically, TRHA performs much better than the two deflated Krylov subspace algorithms *funm_kryl* and *funm_quad*. Similar to the above numerical examples, we remark that the number of matrix-vector products is not the whole story for the matrix exponential problem. For instance, we notice that TRHA used 3005 matrix-vector products and 73.38 seconds, while *expv* used 11036 matrix-vector

products and 74.44 seconds. The reason is that one requires to solve an ODE problem in each outer iteration (cycle) of the TRHA algorithm. Experimentally, we find that if the number of restarting is large, solving the ODE problems during cycles will bring us a large amount of computational overhead.

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